2 7 AUG 20 JC20 Rec'd PCT/PTO FO.M PTO-1390 U.S. DEPARTMENT OF COMMERCE PATENT AND TRADEMARK OFFICE (REV 10-2000) TRANSMITTAL LETTER SO THE UNITED STATES DESIGNATED/ELECTED OFFICE (DO/EO/US) U.S. APPLICATION NO. (If known, see 37 CFR 1.5) **CONCERNING A FILING UNDER 35 U.S.C.371** INTERNATIONAL APPLICATION INTERNATIONAL FILING DATE PCT/SE00/00384 28 February 2000 (28.02.00) 26 February 1999 (26.02.99) TITLE OF INVENTION DRUG DESIGN BASED ON THE STRUCTURE OF LTA4 HYDROLASE APPLICANT(S) FOR DO/EO/US HAEGGSTRÖM, Jesper, Z et al. Applicant herewith submits to the United States Designated/Elected Office (DO/EO/US) the following items and other information: 1. This is a FIRST submission of items concerning a filing under 35 U.S.C.371. 2. This is a SECOND or SUBSEQUENT submission of items concerning a filing under 35 U.S.C. 371. 3. This is an express request to promptly begin national examination procedures (35 U.S.C. 371(f)). 4. The US has been elected by the expiration of 19 months from the priority date (PCT Article 31). 5. A copy of the International Application as filed (35 U.S.C. 371(c)(2)) a. \square is attached hereto (required only if not communicated by the International Bureau). b. 🗷 has been communicated by the International Bureau. c. \square is not required, as the application was filed in the United States Receiving Office (RO/US). 6. An English language translation of the International Application as filed (35 U.S.C 371(c)(2)). 7. Amendments to the claims of the International Application under PCT Article 19 (35 U.S.C. 371(c)(3)) a. \square are attached hereto (required only if not communicated by the International Bureau). b. \square have been communicated by the International Bureau. c. \square have not been made; however, the time limit for making such amendments has NOT expired. d. E have not been made and will not be made. 8. An English language translation of the amendments to the claims under PCT Article 19 (35 U.S.C. 371(c)(3)). 9. An oath or declaration of the inventor(s) (35 U.S.C. 371(c)(4)). (unexecuted) (4 sheets) 10. An English language translation of the annexes to the International Preliminary Examination Report under PCT Article 36 (35 U.S.C. 371(c)(5)). Items 11. to 16. below concern document(s) or information included: 11. An Information Disclosure Statement under 37 CFR 1.97 and 1.98. 12. An assignment document for recording. A separate cover sheet in compliance with 37 CFR 3.28 and 3.31 is 13. A FIRST preliminary amendment. (12 sheets) (along with version of markings to show changes) ☐ A SECOND or SUBSEQUENT preliminary amendment. 14. A substitute specification. 15. A change of power of attorney and/or address letter. 16. Dither items or information: Transmittal Letter (2 sheets in duplicate); International Application Published Under the PCT (with attached International Search Report) WO 00/50577 (156 sheets); PCT International Preliminary Examination Report (6 sheets); Certificate of Express Mailing (1 sheet); and return postcard receipt.

of the second	* * *		ປີເປີລີ ຄະວຸນ :	(Lap 10 2 /	AUG 2001
U.S. APPLICATION NO. (if)	known, see 37 CFR 1.5) 9 1 4 4 5 1	INTERNATIONAL APPL PCT/S	ICATION NO. E00/00384		PVZ-006US
17. E The following fe	es are submitted:			CALCULATIO	NS PTO USE ONLY
		(1) - (5)) .(a/o Novemb	er 1, 2000):		
BASIC NATIONAL FEE (37 CFR 1.492 (a) (1) - (5)).(a/o November 1, 2000): Neither international preliminary examination fee (37 CFR 1.482) nor international search fee (37 CFR 1.445(a)(2)) paid to USPTO and International Search Report not prepared by the EPO or JPO\$1000			<i>3</i> *		
		(37 CFR 1.482) not paid epared by the EPO or JI			
		(37 CFR 1.482) not paid 2)) paid to USPTO			
		paid to USPTO (37 CFF PCT Article 33(1)-(4)			
		paid to USPTO (37 CFF Article 33(1)-(4)			
				\$1,000.00	
e , ty e	ENTER APPROPE	RIATE BASIC FEE A	MOUNT =		
Surcharge of \$130.00 formonths from the earliest	or furnishing the oath or	declaration later than	፷ 20 □ 30	\$130.00	
CLAIMS	NUMBER FILED	NUMBER EXTRA	RATE		1
Total claims	50- 20 =	30	X \$18.00	\$ 540.00	
Independent claims	5 -3 =	2	X \$80.00	\$ 160.00	
MULTIPLE DEPEN	NDENT CLAIM(S) (if		+ 270.00	\$ 270.00	
15 m	TOTAL OF AB	OVE CALCULATION	NS =	\$2,100.00	
14 T	mall entity status. See	37 CFR 1.27. The fees	indicated above	\$1,050.00	
\$= £<		SUBTOTA	L =	\$1,050.00	
Processing fee of \$130.00 for furnishing the English translation later than \(\sum 20 \subseteq 30 \) Fronths from the earliest claimed priority date (37 CFR 1.492(f)).			\$,	
		OTAL NATIONAL	FEE =	\$1,050.00	
Fee for recording the enclosed assignment (37 CFR 1.21(h)). The assignment must be				\$	
		AL FEES ENCLOSI		\$1,050.00	
				Amount to be:	\$
				refunded charged	\$
,				chargeu	3
a. A check in the amount of \$ to cover the above fees is enclosed.					
b. Please charge my Deposit Account No. 12-0080 in the amount of \$1,050.00 to cover the above fees. A duplicate copy of this sheet is enclosed.					
c. E The Commissioner is hereby authorized to charge any additional fees which may be required, or credit					
any overpayment to Deposit Account No. 12-0080 . A duplicate copy of this sheet is enclosed.					
NOTE: Where an appropriate time limit under 37 CFR 1.494 or 1.495 has not been met, a petition to revive (37 CFR 1.137(a) or (b)) must be filed and granted to restore the application to pending status.					
(η_{α})					
SEND ALL CORRESPONDENCE TO SIGNATURE					
Elizabeth A. Hanley, Esq. SIGNATURE LAHIVE & COCKFIELD, LLP Elizabeth A. Hanley					
28 State Street NAME					
Boston, Massachusetts		33,50	5		
United States of Amer	rica	REGIST	RATION NUMBER	-	
(617) 227-7400 Dated: 27 August 2001					

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE



In re the application of: Jasper Haeggström et al.

Serial No.: 09/914,451

Priority Date: February 26, 1999

PCT Filing Date: February 28, 2000 (PCT)

U.S. Filing Date: August 27, 2001

For: "Drug Design Based on the Structure of

LTA4 Hydrolase"

Attorney Docket No.: PVZ-006US

Commissioner for Patents BOX SEQUENCE LISTING Washington, D.C. 20231 Group Art Unit: Not Yet Assigned

Examiner: Not Yet Assigned

TRANSMITTAL LETTER FOR DISKETTE CONTAINING SEQUENCE LISTING

Dear Sir:

1 s

 Responsive to the Notification of Missing Requirements Under 35 U.S.C. §371 in the United States Designated/Elected Office (DO/EO/US) dated October 22, 2001, Applicants' attorney submits a diskette containing a computer readable form of the Sequence Listing for the patent application filed on August 27, 2001. The Sequence Listing complies with the requirements of 37 C.F.R. §1.821-1.825. The material on the enclosed diskette is identical in substance to the Sequence Listing appearing on substitute pages 1 and 2 submitted herewith. The computer readable form of the Sequence Listing contained on the enclosed diskette is understood to comply with the requirements of §1.824(d).

"Express Mail" mailing label number_	EL 892 198 215 US
Date of Deposit	December 20, 2001
Postal Service "Express Mail Post Office	ve and is addressed to the Commissioner

Date: December 20, 2001

Respectfully submitted.

LAHIVE & COCKFIELD, LLP

By:

Elizabeth A. Harley Esq Registration No. 33,505 Attorney for Applicants

IN THE UNITED STATES PATENT DESIGNATED OFFICE (DO/US) (National Phase of International App.: PCT/SE00/00384, WO 00/50577)

In re the

application of: Jesper Z. HAEGGSTRÖM et al.

International Application No.: PCT/SE00/00384

International Filing Date: 28 February 2000

U.S. Serial No.: Not Yet Assigned

Filed: Herewith

For: DRUG DESIGN BASED ON THE STRUCTURE OF LTA₄ HYDROLASE

Attorney Docket No.: PVZ-006US

BOX PCT

Commissioner for Patents Washington, D.C. 20231

PRELIMINARY AMENDMENT

Dear Sir:

Preliminary to examination of the above-referenced patent application, please amend the enclosed above-titled International patent application as follows.

In the Claims

Please amend claims 6, 9, 11, 13, 14, 15, 18, 19, 25, 28, 30, and 35 as follows.

- 6. (Amended) A compound which is substantially complementary to a protein according to claim 1.
- 9. (Amended) An isolated complex, which is comprised of a protein according to claim 1 and a complementary compound according to claim 6, wherein the three-

dimensional structure of LTA₄ hydrolase is essentially as disclosed in Table 9 by the parameters defining atom 1- atom 4876, or a functionally equivalent part, derivative or conformational analogue of such a complex.

- 11. (Amended) Use of the parameters of a protein according to claim 1, a compound according to claim 6 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry.
- 13. (Amended) Use according to claim 11, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or allergic symptoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS).
- 14. (Amended) Use according to claim 11, wherein said drug is for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer.
- 15. (Amended) Use according to claim 11, wherein said drug is for the treatment and/or prevention of disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 18. (Amended) A method according to claim 16, wherein an enzymatic inhibitor complementary to the amino acids defined in claim 3 is screened for.
- 19. (Amended) An analogue obtainable by the method of claim 16.
- 25. (Amended) A compound obtainable by the method according to claim 21.

- 28. (Amended) A process for the purification of a protein according to claim 1 or obtained according to claim 26, which purification includes hydroxyapatite-based chromatography and a subsequent anion exchange chromatography.
- 30. (Amended) A protein obtained by the method according to claim 26.
- 35. (Amended) A protein according to any one of claims 6, 25, 30 or 31 for use as a medicament.

Please cancel claims 36-38.

REMARKS

Applicant amends the claims to remove multiple dependencies, to provide proper antecedent basis, and to address other matters of form. The foregoing amendments introduce no new matter and are not related to issues of patentability.

Entry of the foregoing Preliminary Amendment is respectfully in order and requested.

Attached hereto as Appendix A is a marked-up version of the changes made to the claims by the current amendments. Appendix A is captioned "Version With Markings To Show Changes Made." Also attached hereto as Appendix B is a complete set of the claims that will be pending upon entry of the amendments presented herein.

If there are any questions regarding the amendments to the application, we invite the Examiner to call Applicant's representative at the telephone number below.

Respectfully submitted,

LAHIVE & COCKFIELD, LLP

Registration No. 33,506 Attorney for Applicants

28 State Street Boston, MA 02109 (617) 227-7400

Date: 27 August 2001

APPENDIX A

VERSION WITH MARKINGS TO SHOW CHANGES MADE

In the Claims

Please amend claims 6, 9, 11, 13, 14, 15, 18, 19, 25, 28, 30, and 35 as follows.

- 6. (Amended) A compound which is substantially complementary to a protein according to any one of claims 1-5.
- 9. (Amended) An isolated complex, which is comprised of a protein according to claims 1-5 and a complementary compound according to any one of claims 6-8, wherein the three-dimensional structure of LTA₄ hydrolase is essentially as disclosed in Table 9 by the parameters defining atom 1- atom 4876, or a functionally equivalent part, derivative or conformational analogue of such a complex.
- 11. (Amended) Use of the parameters of a protein according to any one of claims 1-5, a compound according to any one of claims 6-8 or a complex according to claim 9 or 10 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry.
- 13. (Amended) Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or allergic symptoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS).
- 14. (Amended) Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer.

- 15. (Amended) Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 18. (Amended) A method according to claim 16 or 17, wherein an enzymatic inhibitor complementary to the amino acids defined in any one of claims 3, 4 or 5 is screened for.
- 19. (Amended) An analogue obtainable by the method according to any one of claims 16-18.
- 25. (Amended) A compound obtainable by the method according to any one of claims 21-24.
- 28. (Amended) A process for the purification of a protein according to any one of claims 1-3 or obtained according to claim 26-or 27, which purification includes hydroxyapatite-based chromatography and a subsequent anion exchange chromatography.
- 30. (Amended) A protein obtained by the method according to any one of claims 27-29 26.
- 35. (Amended) A protein according to any one of claims 6-8, 25, 30 or 31 for use as a medicament.

APPENDIX B

- 1. An isolated protein comprising at least a subsequence of the amino acid sequence of LTA₄ hydrolase, which exhibits a three-dimensional form essentially as disclosed in Table 9 by the parameters defining atom 1 to atom 4876, said subsequence being capable of participating in the control of the enzymatic pathway, such as the leukotriene cascade, or a functionally equivalent part, derivative or conformational analogue thereof.
- 2. A protein according to claim 1, which comprises an enzymatically active site defined in the following table:

	Left Wall	Right Wall
1		Lys608, Asp606, Lys605, Lys354, Thr355
2	Phe356, Phe362	Gln544, Asp573, Lys572, Arg568
3	Val376	Lys565, Arg540, Leu507
4	Ser380, Ser352, Glu348	Pro569
5	Tyr378, Glu348	Arg563, Glu533, Phe536, Arg537, Tyr267
6	Tyr383, Phe314, Glu318, Glu384, Arg326	g: 13, 13000,1 Moos 0,1 Mg551, 1 J1201
7	Gly268, Gly269, Met270	His295, Asn341, Phe340
8	Ser288, His497	Glu325, Asn291

- 3. A protein according to claim 2, which is an enzyme having a metallohydrolase activity capable of participating in the regulation of enzyme activities in biochemical pathways, wherein said enzymes have structures similar to the ones defined in claim 2.
- 4. A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Glu318; Tyr378; Tyr383; Arg563; Lys565.
- 5. A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Va1292; His295; Glu296; His299; Trp315; Glu318; Val322; Phe362; Va1367; Leu369; Pro374; Asp375; Ile372; Ala377; Pro382; Tyr378; Tyr383; Arg563; Lys565.

- 6. A compound which is substantially complementary to a protein according to claim 1.
- 7. A compound according to claim 6, which is substantially complementary to an enzymatically active site of said protein and which is capable of specifically inhibiting said enzymatic activity.
- 8. A compound according to claim 7, which is an inhibitor of a metallohydrolase enzyme.
- 9. An isolated complex, which is comprised of a protein according to claim 1 and a complementary compound according to claim 6, wherein the three-dimensional structure of LTA₄ hydrolase is essentially as disclosed in Table 9 by the parameters defining atom 1- atom 4876, or a functionally equivalent part, derivative or conformational analogue of such a complex.
- 10. A complex according to claim 9, wherein the protein complexed with LTA₄ hydrolase is selected from the group which consists of bestatin, thiolamine or hydroxamic acid or a functionally equivalent part, derivative or conformational analogue of such a complex.
- 11. Use of the parameters of a protein according to claim 1, a compound according to claim 6 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry.
- 12. Use according to claim 11, wherein said parameters are selected from the parameters disclosed in Table 9 defining atom 1- atom 4876.

- 13. Use according to claim 11, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or allergic symptoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS).
- 14. Use according to claim 11, wherein said drug is for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer.
- 15. Use according to claim 11, wherein said drug is for the treatment and/or prevention of disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 16. A method for screening LTA₄ hydrolase hydrolase analogues that mimic at least a part of 5 the three-dimensional structure of the LTA₄ hydrolase molecule as defined by the parameters shown in Table 9 for atom 1 to atom 4876, which comprises the steps of
- (a) producing a multiplicity of analogue structures of LTA₄ hydrolase and
- (b) selecting an analogue structure, wherein the three-dimensional configuration and spatial arrangement of one or more enzymatically active sites and/or binding sites of said LTA₄ hydrolase remain substantially preserved.
- 17. A method according to claim 16, wherein an analogue exhibiting an enzymatic activity, such as an epoxide hydrolase and/or aminopeptidase activity, is selected.
- 18. A method according to claim 16, wherein an enzymatic inhibitor complementary to the amino acids defined in claim 3 is screened for.
- 19. An analogue obtainable by the method of claim 16.

- 20. An analogue according to claim 19, which exhibits an increased catalytic activity when compared to the naturally occurring form of LTA₄ hydrolase, such as defined in Table 9 by parameters of atom 1 to atom 4876.
- 21. A method for screening LTA₄ hydrolase binding compounds complementary to a region of LTA₄ hydrolase, preferably an enzymatically active site thereof, which comprises the steps of
- (a) producing a multiplicity of possible complementary structures and
- (b) selecting a structure, wherein the three-dimensional configuration and spatial arrangement of regions involved in binding to LTA₄ hydrolase remain substantially preserved, which selection is based on the three-dimensional structure of LTA₄ hydrolase, and/or LTA₄ hydrolase complexed to an inhibitor thereof, in a form adopted thereof in nature, such as defined in Table 9.
- 22. A method according to claim 21, wherein a general metallohydrolase inhibitor is selected, which is capable of inhibiting an enzyme belonging to the M1 family.
- 23. A method according to claim 21, wherein an inhibitor of the epoxide hydrolase activity and/or aminopeptidase activity of LTA₄ hydrolase or of LTA₄ syntheses is selected.
- 24. A method according to claim 21, wherein a compound capable of antagonizing LTB₄ receptor binding of a cell is selected.
- 25. A compound obtainable by the method according to claim 21.
- 26. A method of engineering a protein, which method comprises the steps of
- identification of a suitable set of mutations based on the structure of LTA₄ hydrolase;
- generation of a library of genes which contains the suitable sequence variations;

- selection of clones encoding the LTA₄ hydrolase analogues with a desired activity function;

wherein said desired activity is the capability of efficiently producing an organic compound of interest.

- 27. A method according to claim 26, wherein the specified property is the suicidal mode of action of LTA₄ hydrolase.
- 28. A process for the purification of a protein according to claim 1 or obtained according to claim 26, which purification includes hydroxyapatite-based chromatography and a subsequent anion exchange chromatography.
- 29. A process for the crystallization of an LTA₄ hydrolase, an analogue or a derivative thereof, wherein said crystallisation is performed with the addition of an ytterbium salt as an additive, such as an ytterbium chloride.
- 30. A protein obtained by the method according to claim 26.
- 31. A protein according to claim 30, which is present in an essentially pure form.
- 32. An isolated nucleic acid encoding a protein according to claim 30 or 31.
- 33. A nucleic acid capable of specifically hybridising to a nucleic acid according to claim 32.
- 34. Use of a protein, which is a genetically modified LTA₄ hydrolase, according to claim 30 or 31 in the preparation of LTB₄ or other metabolites in the leukotriene cascade.
- 35. A protein according to any one of claims 6, 25, 30 or 31 for use as a medicament.

WO 00/50577

PCT/SE00/00384

DRUG DESIGN BASED ON THE STRUCTURE OF LTA4 HYDROLASE

1. BACKGROUND

1.1 Technical field

The present invention relates to methods of design or identification of biologically active compounds, which methods are based on the first definition ever of a three-dimensional structure of a protein involved in the leukotriene cascade. Further, the invention relates to novel compounds obtained by said methods, to advantageous uses of such compounds as well as to processes for the preparation thereof.

1.2 Prior art

Leukotriene A4 (LTA₄) hydrolase is a pivotal enzyme in the biosynthesis of leukotrienes, a family of paracrine hormones implicated in the pathophysiology of inflammatory and allergic disorders, in particular bronchial asthma (Samuelsson, B. Science 220, 568-75 (1983); and Lewis, R.A., Austen, K.F. & Soberman, R.J. N Engl J Med 323, 645-55 (1990)). Leukotrienes are formed by immunocompetent cells including neutrophils, eosinophils, basophils, mast cells, and macrophages, in response to a variety of immunological as well as non-immunological stimuli. These lipid mediators are divided into two major classes exemplified by the chemotaxin LTB4, and the spasmogenic cysteinyl-leukotrienes (LTC4, LTD4, and LTE4). Leukotriene biosynthesis is initiated by the enzyme 5-lipoxygenase which converts arachidonic acid into the unstable epoxide LTA4, a central intermediate in the leukotriene cascade. LTA4 may in turn be hydrolyzed into LTB4 by the enzyme LTA4 hydrolase, or conjugated with GSH to form LTC4, a reaction catalyzed by a specific LTC4 synthase. During cellular activation, all key enzymes in leukotriene biosynthesis, except LTA4 hydrolase, form a biosynthetic complex assembled at the nuclear membrane, suggesting that leukotrienes may have unknown intranuclear functions related to gene regulation or cell growth (Serhan, C.N., Haeggstrom, J.Z. & Leslie, C.C. Faseb J 10, 1147-58 (1996)).

Leukotriene B4, the natural product of LTA4 hydrolase, is one of the most powerful chemotactic agents known to date and triggers leukocyte adherence and ag-

5

20

25

25

5

gregation at only nM concentrations (Ford-Hutchinson, A.W., Bray, M.A., Doig, M.V., Shipley, M.E. & Smith, M.J.H. Nature 286, 264-265 (1980)). Hence, this molecule is regarded as a key mediator of inflammation, and has been implicated in a number of diseases, including arthritis, psoriasis, inflammatory bowel disease (IBD), and chronic obstructive pulmonary disease (COPD). Furthermore, the role of LTB4 in inflammation has been well corroborated by the anti-inflammatory properties of LTA4 hydrolase inhibitors, particularly in combination with a cyclooxygenase inhibitor, and specific LTB4 receptor antagonists, as well as the reduced inflammatory reactions observed in several animal models of leukotriene deficiency (Tsuji, F., Miyake, Y., Enomoto, H., Horiuchi, M., Mita, S. Eur. J. Pharmacol. 346, 81-85, (1998); Chen, X.S., Sheller, J.R., Johnson, E.N. & Funk, C.D. Nature 372, 179-182 (1994); Griffiths, R.J., et al. Proc Natl Acad Sci USA 92, 517-21 (1995); and Griffiths, R.J., et al. J Exp Med 185, 1123-9 (1997)). In addition, LTB4 modulates the immune response, e.g., by interference with specific subsets of lymphocytes, production of cytokines, as well as liberation of immunoglobulins from B-lymphocytes (Payan, D.G., Missirian-Bastian, A. & Goetzl, E.J. Proc Natl Acad Sci U S A 81. 3501-5 (1984); Rola-Pleszczynski, M. & Lemaire, I. J Immunol 135, 3958-61 (1985); and Yamaoka, K.A., Claesson, H.E. & Rosen, A. J. Immunol 143, 1996-2000 (1989)). Recent data also indicate that LTB4 stimulates, and thus has a crucial role in the regulation of, cell proliferation and cell survival in HL-60 cells, suggesting that LTA4 hydrolase inhibitors may have an anti-proliferative effect. (Dittman, K.H., Mayer, C., Rodemann, H.P., Petrides, P.E., and Denzlinger, C. Leuk, Res. 22. 49-53 (1998)). The cell surface receptor for LTB4 (BLTR) was recently cloned and found to be abundantly expressed in the immune system, including lymphocytes, spleen and thymus (Yokomizo, T., Izumi, T., Chang, K., Takuwa, Y. & Shimuzu, T. Nature 387, 620-624 (1997)). BLTR belongs to a family of chemokine receptors and, interestingly, together with CD4 it was found to be an efficient coreceptor for HIV-1 infection (Owman, C., et al. Proc Natl Acad Sci USA 95, 9530-4 (1998)). Moreover, LTB4 is also a natural ligand to the nuclear orphan receptor PPARa.

25

5

suggesting that LTB4 may have intranuclear functions possibly related to lipid homeostasis (Devchand, P.R., et al. Nature 384, 39-43 (1996)).

LTA4 hydrolase is a cytosolic 69 kDa enzyme without any similarity to other soluble or membrane bound xenobiotic epoxide hydrolases (Funk, C.D., et al. Proc Natl Acad Sci U S A 84, 6677-81 (1987)). The enzyme's epoxide hydrolase activity, which generates LTB4, is highly substrate selective accepting only LTA4 and to a small extent the double bond isomers LTA3 and LTA5. Typically, LTA4 hydrolase undergoes suicide inactivation and covalent modification when exposed to LTA4 (Evans, J.F., Nathaniel, D.J., Zamboni, R.J. & Ford-Hutchinson, A.W. J. Biol. Chem. 260, 10966-10970 (1985)). During this process, LTA4 apparently binds to Tyr-378, a residue which also seems to play a role for the formation of the critical cis-trans-trans geometry in the conjugated triene structure of LTB4 (Mueller, M.J., et al. Proc Natl Acad Sci U S A 93, 5931-5935 (1996); and Mueller, M., Andberg, M., Samuelsson, B. & Haeggstrom, J. Z. J. Biol. Chem. 271, 24345-24348 (1996)).

From sequence comparisons with certain metalloproteases and aminopeptidases, a zinc binding motif (HEXXH-X18-E) was unexpectedly found in LTA4 hydrolase (Vallee, B.L. & Auld, D.S. Proc. Natl. Acad. Sci. USA 87, 220-224 (1990)). Further studies demonstrated that the enzyme indeed contains one catalytic zinc atom complexed to His295, His299, and Glu318 (Medina, J.F., et al. Proc. Natl. Acad. Sci. USA 88, 7620-7624 (1991)). In addition, a previously unknown peptide cleaving activity was discovered which requires the presence of anions, particularly chloride (Haeggström, J.Z., Wetterholm, A., Medina, J.F. & Samuelsson, B. J Lipid Mediator 6, 1-13 (1993)). Although the endogenous physiological peptidase substrate(s) has not yet been identified, LTA4 hydrolase cleaves certain arginyl di- and tripeptides with very high efficiency (Örning, L., Gierse, J.K. & Fitzpatrick, F.A. J. Biol. Chem. 269, 11269-11273 (1994)). Hence, LTA4 hydrolase can be described as a bifunctional zinc metalloenzyme with the unique ability to accept both lipid and peptide substrates. Using site-directed mutagenesis, Glu296 and Tyr383 were found to be critical for the peptidase reaction, presumably as a general base and proton donor, respectively (Blomster, M., Wetterholm, A., Mueller, M.J. & Haegeström

5

J.Z. Eur. J. Biochem. 231, 528-534 (1995); and Wetterholm, A., et al. Proc Natl Acad Sci U SA 89, 9141-9145 (1992)). Since the enzyme's ability to convert LTA4 into LTB4 was not affected by the mutations, the two enzyme activities of LTA4 hydrolase are exerted via non-identical but overlapping active sites. Notably, unlike other enzymes in the leukotriene cascade, LTA4 hydrolase is ubiquitous in mammalian cells and tissues suggesting that it may have other functions presumably related to its peptide cleaving activity.

As a consequence of the identification of LTA₄ hydrolase as a zinc metalloen-zyme with a peptidase activity, it was observed that LTA₄ hydrolase is inhibited by bestatin, a general aminopeptidase inhibitor, and captopril, an inhibitor of angiotensin converting enzyme (Örning, L., et al. J. Biol. Chem. 266, 16507-16511 (1991)).

Tsuge et al., (J. Mol. Biol. 238,854-856 (1994)), have described the crystallization of LTA₄ hydrolase. However, despite the well recognized need thereof, the three-dimensional structure of LTA4 hydrolase has not yet been disclosed. More specifically, the problems that need to be overcome in order to provide such a determination may in brief be explained as follows. There are two major difficulties in obtaining a three-dimensional structure of a protein molecule. The first one is to grow crystals of good quality that are reproducible and diffract to atomic resolution (beyond 2.5Å). This means a thorough and cumbersome investigation of parameters that influence the crystal growth such as pH, temperature, nature of buffers, nature of precipitant, just to mention a few. The addition of ligands such as substrate analogues or inhibitors or the addition of other molecules can be important for obtaining good crystals. There is only little understanding of the physical background of the crystallisation process which means that the search for suitable crystallisation conditions for a certain protein is unique, requires creativity and intuition, and is governed by trial and error procedures. The purity of the protein is also a crucial parameter in the crystallisation and a suitable degree of purity can be hard, or even imposible, to achieve. The second major difficulty is associated with overcoming the phase-problem which is inherent to X-ray diffraction methods. To be able to overcome this problem it is necessary to substitute the protein with suitable heavy

5

atom substance such as e.g. mercury, gold or platinum compounds. Crystals often cannot withstand the treatment with these compounds and the search for suitable substitutions is not straight forward and may become very exhaustive. Another option is to substitute all methionines by seleno-methionine (Se-Met) residues. This method requires production of recombinant protein in special strains of E. coli under non-standard conditions, followed by a new purification and recrystallisation of the Se-Met containing protein. Although Tsuge et al reported the crystallisation of LTA4 hydrolase, their crystals only diffracted to medium resolution and the phaseproblem was not solved. Thus, as a reliable definition of the three-dimensional structure of LTA₄ hydrolase would enable e.g. a display in visual form on a computer screen of the shape of the molecule, then, could the above mentioned problems be solved, a whole range of possibilities would be opened, such as rational structure-based drug design, e.g. in combination with combinatorial chemistry, aimed at production of novel medicaments useful in disorders associated with the leukotriene cascade, as well as protein-engineering to create novel variants of the enzyme with altered, but yet useful, catalytic properties.

As LTA4 hydrolase is a recognized important drug target, some inhibitors thereof have been synthesized (Wetterholm, A., et al. J Pharmacol Exp Ther 275, 31-7 (1995); and Yuan, W., Wong, C., Haeggstrom, J. Z., Wetterholm, A. & Samuelsson, B. J. Am. Chem. Soc., 114, 6552-6553 (1992)). Interestingly, certain inhibitors of LTA4 hydrolase were reported to act also as LTB4 receptor antagonists (Labaudinière R, Hilboll G, Leon-Lomeli A, Terlain B, Cavy F, Parnham M, Kuhl P, and Dereu N. J. Med. Chem. 35, 3170-3179 (1992)). Due to the absence of any available information regarding the three-dimensional structure of LTA4 hydrolase, as discussed above, none of the previously described inhibitors have been designed based on the exact structure thereof. Accordingly, there is a need within this field of determining the three-dimensional structure of LTA4 hydrolase in order to design more potent and selective inhibitors of LTA4 hydrolase as well as modified structures exhibiting even more advantageous pharmaceutical properties.

2. THE PRESENT INVENTION

As the following chapter includes a substantial amount of text, it has herein been divided into separate sections, each one of which disclose separate aspects of the present invention.

5

1.15

20

25

30

2.4.8 (a) Method

2.4.8. (b) Novel specifically designed proteins

2.4.8. (c) Use of genetically modified LTA₄ hydrolase

Index Chapter 2
2.1 Summary of the invention
2.2 Brief description of the drawings
2.3 Definitions
2.4 Detailed description of the invention
2.4.1 LTA ₄ hydrolase, subsequences and analogues thereof
2.4.2 Compounds complementary to LTA ₄ hydrolase
2.4.3 A complex of LTA ₄ hydrolase and acomplementary compound
2.4.4 Advantageous uses of LTA ₄ hydrolase, complementery compounds and
complexes thereof
2.4.5 Screening for LTA ₄ hydrolase analogues
2.4.5 (a) Method
2.4.5 (b) Analogues obtainable by the present screening method
2.4.5 (c) Mutated forms of LTA ₄ hydrolase obtainable by the present screening
method
2.4.5 (d) Nucleic acids encoding the novel compounds
2.4.6 (a) Production and purification of genetically modified forms of LTA ₄
hydrolase
2.4.6 (b) Purified LTA ₄ hydrolase
2.4.7 Identification of LTA ₄ hydrolase binding compounds
2.4.7 (a) Method
2.4.7 (b) Identified binding compounds
2.4.8 Protein engineering

- 2.4.9 Pharmaceutical applications of the present invention
- 2.4.9 (a) First medical indication
- 2.4.9 (b) Second medical indication and pharmaceutical methods
- 2.4.9.(c) Methods of treatment
- 5 2.5 Production of the novel molecules
 - 2.6 Detailed description of the drawings

2.1 Summary of the invention

The object of the present invention is to fulfill the above defined need. This has been achieved by the crystallization and determination of the three-dimensional structure of LTA4 hydrolase complexed with the competitive inhibitor bestatin and subsequent structure determination of complexes between LTA4 hydrolase and two specific inhibitors. It is the first three-dimensional structure of any protein component of the leukotriene cascade and enables a description of the structural basis and molecular mechanisms of various enzyme functions, such as the two catalytic activities of LTA4 hydrolase. In addition, the structural information will now make possible rational design of enzyme inhibitors, which may be developed into clinically useful anti-inflammatory drugs.

2.2 Brief description of the drawings

Figure 1 shows the key enzymes and intermediates in leukotriene biosynthesis.

Figure 2 shows 2Fo-Fc density contoured at 1.1 s. Part of the active site in the neighborhood of the bestatin molecules is shown.

Figure 3 is a ribbon diagram of the tertiary structure of leukotriene A4 hydrolase.

Figure 4 shows ribbon diagrams of the N-terminal domains of . LTA₄ hydrolase.

Figure 5 shows ribbon diagrams of the catalytic domain of LTA₄ hydrolase and therolysin.

Figure 6 shows the structure of the C-terminal domain.

Figure 7 illustrates zinc binding ligands in LTA4 hydrolase.

Figure 8 (a) is a Ball-and-Stick presentation of the binding of bestatin in LTA4 hydrolase, while Figure 8 (b) is a schematic overview of bestatin binding in LTA4 hydrolase.

Figure 9 (a) is a wire representation of the central cavity found in LTA4 hydrolase (shown as $C\alpha$ -trace).

Figure 9 (b) is a schematic presentation for the proposed binding of LTA4 into the cavity.

Figure 10 is a schematic representation for the proposed reaction mechanism of the epoxide hydrolase.

2.3 Definitions

In the present context, the term "the three-dimensional form adopted thereof in nature" is to be understood as the conformational structure, defined by the parameters x, y and z in a conventional coordinate system, that a naturally occurring molecule adapt under conditions where it is capable of exerting its biological activities.

The specific conditions during which the herein presented data were collected are detailed in the section "Experimental".

The term "isolated" and variations thereof when used in connection with a molecule, such as protein, a polypeptide or a nucleic acid, means that said molecule is isolated from other substances, such as other proteins, DNA etc normally accompanying it in its natural environment.

The term "leukotriene A₄ (LTA₄) hydrolase" as used herein is to be understood to include any mammalian or other LTA₄ hydrolase which comprises the same backbone as the human form specifically disclosed in the present application, irrespective of source. The amino acid sequences of mammalian LTA4 hydrolase have been shown to be identical to about 90%. Thus, the three-dimensional structures thereof may be suspected to be identical to approximately the same extent.

"Thiolamine" and "hydroxamic acid" are used herein to denote the compounds examplified in the Experimental section of the present specification.

A "complementary compound" means any compound, the structure of which enables a binding thereof to a specified protein, i.e a compound having a conformation or structure enabling such a suitable fit as to provide an energetically favorable interaction between protein-complementary compound.

20

25

5

"Analogue" means, as used herein, a chemically altered molecule which shares the backbone with, or at least structurally resembles, a "parent molecule". In the present specification, such a "parent molecule" may be LTA₄ hydrolase or an inhibitor thereof.

In the present application, the term "active site" is to be understood to include any region capable of binding a substrate and converting it into product.

The term "nucleic acid" refers to a deoxyribonucleotide or ribonucleotide polymer in either single- or double-stranded form, and unless otherwise limited, encompasses known analogs of nucleotides, that can function in a similar manner as naturally occurring nucleotides.

The phrase "hybridising specifically to" refers to the binding, duplexing, or hybridising of a molecule only to a particular nucleotide sequence under stringent conditions when that sequence is present in a complex mixture (e.g., total cellular) of DNA or RNA. The term "stringent conditions" refers to conditions under which a probe will hybridise to its target subsequence, but to no other sequences. Stringent conditions are sequence-dependent and will be different in different circumstances. Longer sequences hybridise specifically at higher temperatures. Generally, stringent conditions are selected to be about 5°C lower than the thermal melting point Tm for the specific sequence at a defined ionic strength and pH. The Tm is the temperature (under defined ionic strength, pH, and nucleic acid concentration) at which 50% of the probes complementary to the target sequence hybridise to the target sequence at equilibrium. (As the target sequences are generally present in excess, at Tm, 50% of the probes are occupies at equilibrium). Typically, stringent conditions will be those in which the salt concentration is less than about 1.0 M Na ion, typically about 0.01 to 1.0 M Na ion concentration (or other salts) at pH 7.0 to 8.3 and the temperature is at least about 30°C for short probes (e.g., 10 to 50 nucleotides) and at least about 60°C for long probes (e.g., greater than 50 nucleotides). Stringent conditions may also be achieved with the addition of destabilizing agents such as formamide.

"Essentially pure" means herein a purity of at least about 80%, especially at least about 90% and preferably at least about 95%, such as 98-99%. The purity of

25

30

5

LTA₄ hydrolase, an analogue or inhibitor thereof is according to the present invention preferably determined by general biochemical and biophysical methods well-known to the skilled in this field. For proteins, SDS polyacrylamide gel electrophoresis (SDS-PAGE) with Coomassie and silver staining or amino acid sequence analysis can be used, whereas high-pressure liquid chromatography (HPLC), gas chromatography coupled to mass spectrometry (GC-MS), and nuclear magnetic resonance spectroscopy (NMR) are suitable methods for small organic molecules (peptides, lipids, or carbohydrates, or combinations of these classes of substances).

2.4 Detailed description of the invention

2.4.1 LTA₄ hydrolase, subsequences and analogues thereof

In a first aspect, the present invention relates to an isolated protein comprising at least a subsequence of the amino acid sequence of leukotriene A₄ (LTA₄) hydrolase, which subsequence has the corresponding three-dimensional form adopted thereof in nature. The protein according to invention as discussed below and elsewhere in this application is also understood to encompass any other functionally equivalent part, derivative or conformational analogue thereof. More specifically, the invention relates to the above disclosed protein which comprises a subsequence of the amino acid sequence of leukotriene A₄ (LTA₄) hydrolase, which is able to participate in, and influence, e.g. by providing enzymatic activity, the leukotriene cascade. Most preferably, the protein according to the invention is capable of controling said cascade by exerting an enzymatic activity and thus regulate the production of leukotriene B₄ (LTB₄). In a particular embodiment, the protein is comprised of essentially all of the amino acid sequence of leukotriene A₄ (LTA₄) hydrolase as disclosed in SEQ ID NO 1, or a functionally equivalent part, derivative or conformational analogue thereof.

Thus, the present invention relates to an isolated LTA₄ hydrolase in its naturally ocurring three-dimensional form. More specifically, the present application provides a listing illustrating, for the first time, the coordinates defining human LTA₄ hydrolase complexed to an inhibitor thereof. Thus, the coordinates defining the conformation of LTA₄ hydrolase have been determined by the present inventors as com-

plexed with bestatin, thiolamine and hydroxamic acid, respectively. Bestatin is a

5

25

30

20

universal inhibitor of amino peptidase activity (see e.g. Mathé, G. Biochem. Pharmacol. 45, 49-54 (1991)), while the last mentioned two are specific inhibitors of LTA₄ hydrolase. Based on these different activities, said inhibitors may be used as models in the design of novel molecules having desired properties. Methods for such design will be discussed in further detail below as a further advantageous aspect of the invention. For reasons of convenience for the reader of the present specification, the data collection comprising the novel coordinates according to the invention is included in the present description as a separate section denoted "X-ray data", as Table 9, immediately preceding the claims. In said table, atom no 1 to atom no 4876 define the LTA₄ hydrolase part of the complex. (protein part), atom no 4877 refers to Zn, atom nos. 4878-4880 refer to Yb, atom nos. 4881-4885 refer to imidazole, atom nos. 4886-4889 refer to acetate, atom nos 4890-4908 refer to thiolamine while atom nos. 4909-5160 refer to water. Thus, the intervening atoms relate to the metals that bind in LTA₄ hydrolase, i.e. the active site Zn atom and the Yb atoms that were crucial for the present structure determination. The conditions prevailing at the determination thereof will be described in detail in the Experimental section below. As the skilled in this field realises, such coordinates usually exhibit a certain degree of variation, due to e.g. thermal motion and slight differences in crystal packing. Thus, any references herein to Table 9 in connection with the proteins and other molecules are merely intended to illustrate an average value for each of the coordinates defining the conformation of the molecules under identical conditions, as determined by use of the same apparatus and method. Accordingly, this embodiment of the invention is not limited to a molecule having exactly the specified coordinates, but rather to molecules capable of adopting such a structure. For example, a human LTA₄ hydrolase according to the invention will exhibit a strong bit a conformational similarity with the coordinates presented by atom nos 1 -4876 of Table 9, wherein a variation of about 1%, or 0.5 Å, may be expected. Accordingly, any such variants are within the scope of the present invention.

As regards amino acid sequence, in a specific embodiment, the protein according to the invention is identical, by direct sequence comparison, to at least about

50%, more specifically, at least about 70%, such as at least about 90%, to the LTA₄ hydrolase as defined by SEQ ID NO. 1 while in the three-dimensional form adopted thereof in nature. In this context, it is noted that the amino acid sequence of LTA₄ hydrolase also appears from the data of Table 9, but is also included as a separate sequence listing for reasons of clarity. The protein of this embodiment of the invention are e.g. variants originating from any species, preferably mammals, such as humans, mice or other rodents, etc. Alternatively, the variants including subsequences of the human sequence are mutated forms, resulting from either spontaneous mutations or deliberately produced mutations, as discussed in more detail below.

One preferred embodiment of the present invention is a protein which comprises at least one of the regions defined below in Tables 1-3 below as active sites.

Table 1: Residues lining the big cavity from outsite to insite

	Left wall	Right wall
1	_	Lys608, Asp606, Lys605,
		Lys354, Thr355
2	Phe356, Phe362	Gln544, Asp573, Lys572, Arg568
3	Val376	Lys565, Arg540, Leu507
4	Ser380, Ser352, Glu348	Pro569
5	Tyr378, Glu348	Arg563, Glu533, Phe536,
•		Arg537, Tyr267
6	Tyr383, Phe314, Glu318, Glu384,	
	Arg326	
7	Gly268, Gly269, Met270	His295, Asn341, Phe340
8	Ser288, His497	Glu325, Asn291

15

In Table 1, Lys565, Ser380, Pro569, Glu533, Tyr383, Phe314, Glu318, Glu384, Arg326, Gly268, Gly269, Met270, His295, Phe340, Ser288, and Glu325 are strictly conserved amino acids, while Lys608, Phe356, Phe362, Lys572, Arg568, Tyr378, Phe536, Tyr 267, and Asn291 are conserved in nature.

20

25

30

5

Table 2: Amino-acids in the bestatin binding site ("basic" amino-peptidase site)

The binding of bestatin to LTA₄ hydrolase may also be described by way of coordinates. Below follows the specific amino acids involved in the binding of bestatin and similar structures, as defined according to the invention.

Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Glu318; Tyr378; Tyr383; Arg563; Lys565.

Table 3: Amino acids in the leukotriene binding site

The present amino acids define the site binding leukotriene-based inhibitors, such as thiolamine and hydroxamic acid, as shown in Table 9 for thiolamine.

Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Trp315; Glu318; Val322; Phe362; Val367; Leu369; Pro374; Asp375; Ile372; Ala377; Pro382; Tyr378; Tyr383; Arg563; Lys565.

In Tables 1-3 above, the enumeration of the amino acid sequence of LTA₄ hydrolase begin without the initial Met. Thus, compared to SEQ ID NO 1, which includes the initial Met, the amino acid enumeration above is lowered by one. Accordingly, Gln136 above corresponds to Gln 137 of SED ID NO 1, Ala137 above corresponds to Ala 138 of SEQ ID NO 1, etc.

Table 4: General catalytic domain for the M1 class of enzymes Amino acids no. 210-450.

The present region will provide a basis for the development of enzyme inhibitors useful in the control other biological pathways than the leukotriene cascade.

Thus, as regards the above defined region of aminopeptidase activity of LTA₄ hydrolase, the present inventors have surprisingly observed, that said region is in fact universal for all enzymes belonging to the metallohydrolase family denoted M1.

25

5

Thus, this specific subsequence of LTA₄ hydrolase is encompassed by the present invention as a novel protein *per se*. In addition to the various advantageous uses of subsequences of LTA₄ hydrolase described herein in connection with the leukotriene cascade, this region, which is shared between all M1 enzymes, will find several further applications in connection with other enzymatic pathways. For example, the present region, herein denoted the "M1 region" in order to clarify that it is shared between the M1 enzymes, may advantageously be used to produce synthetic inhibitors, or identify natural inhibitors, of any one of the other M1 enzymes. Such M1 inhibitors will be discussed below when compounds complementary to LTA₄ hydrolase are disclosed.

The above disclosed proteins and peptides comprising subunits of LTA₄ hydrolase are advantageously used e.g. as enzymes or more preferably in methods wherein novel inhibitors of enzymatic activities are identified and/or designed.

2.4.2 Compounds complementary to LTA₄ hydrolase

In a second aspect, the present invention relates to a novel compound defined by a structure substantially complementary to the above described protein, preferably identified by use of the novel LTA₄ hydrolase conformation according to the present invention. The complementary compound is a naturally occurring or synthetic protein, peptide, lipid, carbohydrate or any other organic or inorganic compound. In relation to naturally occurring compounds, it is to be understood that the present invention relates to such compounds as isolated from their natural environment, preferably identifiable by aid of the novel coordinates defining structures according to the invention, as examplified by the complementary compounds used in the complexes shown in Table 9.

In a first embodiment, the present complementary compound is substantially complementary to an enzymatically active site of the protein and is advantageously capable of specifically inhibiting an enzymatic activity of said protein. Thus, in one embodiment, the present compound is substantially complementary to parts, or all, of the "basic" aminopeptidase binding site defined in Table 2 above. Thus, the pres-

25

5

ent compound is an inhibitor capable of specifically inhibiting an aminopeptidase activity of an enzyme, preferably of LTA₄ hydrolase. In an alternative embodiment, the present compound is substantially complementary to parts, or all, of the leukotriene binding site as defined in Table 3 above. Thus, the present compound is an inhibitor capable of specifically inhibiting an epoxide hydrolase activity of an enzyme, preferably of LTA₄ hydrolase. (The inhibition of both aminopeptidase and epoxidase hydrolase is discussed in detail below in the experimental section.) As the present two binding sites of LTA₄ hydrolase overlap in part, a further embodiment is a compound which is complementary to essential parts of both of the above discussed two binding sites, in part or partially, which thus preferably is an inhibitor of both the discussed activities.

As already mentioned above, one compound which is complementary to an enzymatically active site of LTA₄ hydrolase is a compound complementary to the M1 region thereof and thus capable of partial or total inhibition of the enzymatic activity of LTA₄ hydrolase or any other metallohydrolase belonging to the M1 family. In the present application, such inhibitors will be denoted M1 inhibitors.

As the skilled in this field will realise, the present inhibitors disclosed above need not be compound that inhibit a biological activity completely, but may be capable of exerting a partially inhibiting activity, i.e, lowering the enzymatic activity.

In another embodiment, the present complementary compound is a compound which is also capable of binding to the receptor for the product of an LTA₄ hydrolase, i.e. an LTB₄ receptor, e.g. on a cell, such as a polymorphonuclear leukocyte. Thus, such a compound may be useful as an LTB₄ antagonist whereby the biological effect of LTA₄ hydrolase activity may be regulated. Accordingly, any such LTB₄ antagonist designed and/or identified using the coordinates of LTA₄ hydrolase as presented herein are also encompassed by the present invention.

In another embodiment, the present complementary compound is a compound which, apart from being capable of binding to an active site of LTA4 hydrolase, is also capable of binding to an active site of LTC4 synthase which binds the same substrate as LTA4 hydrolase, i.e. LTA4, and turns it over into LTC4 (cf. Fig 1) and

25

5

is thus expected to share important structural features with the active site of LTA4 hydrolase. Such a compound may be useful as an inhibitor of LTC4 biosynthesis, whereby the production thereof may be regulated. Accordingly, any such LTC4 synthase inhibitor, designed and/or identified using the coordinates of LTA4 hydrolase, are also encompassed by the present invention.

The specific properties and advantageous uses of the present compounds as well as the design and production of novel LTA₄ hydrolase inhibitors will be described in further detail below in relation to the various methods.

2.4.3 A complex of LTA₄ hydrolase and a complementary compound

In a third aspect, the present invention relates to an isolated complex comprised of a protein as described above and a compound complementary to said protein. Said complementary compound may thus be an inhibitor of one or more of the protein's enzymatic activities, such as an aminopeptidase and/or epoxide hydrolase activity, such as bestatin, hydroxamic acid or thiolamine, or leukotriene B4 or any analogue thereof, or LTC₄ or any analogue thereof. Examples of complementary compounds are bestatin, thiolamine or hydroxamic acid. In the present context, it is to be understood that the invention also relates to specific regions of said inhibitors. that have never been specifically disclosed for the present purpose, as well as novel inhibitors identified by aid of the present invention. In specific embodiments, the complex according to the invention is composed of LTA₄ hydrolase complexed with bestatin, thiolamine or hydroxamic acid, respectively, wherein the LTA₄ hydrolase is as defined by the coordinates presented in Table 9, or any functional fragment, derivative or analogue thereof. As bestatin is aminopeptidase based, further similar and advantageous inhibitors may be developped based on the structural information for LTA₄ hydrolase complexed with bestatin, preferably combined with the specification of the binding site of Table 2. Further, as both thiolamine is leukotriene based, the information provided in Table 9, preferably combined with the specification of binding site of Table 3, will prove to be an advantageous tool in order to gain more information about such enzymatic binding and thus the development of further

25

5

novel inhibitors, the same principles applying to hydroxamic acid, which is also leukotriene based.

Accordingly, the present invention presents for the first time the coordinates defining the three-dimensional structure of a complex of LTA₄ hydrolase and an inhibitor thereof as determined by X-ray crystallography, e.g. as illustrated in Table 9. In fact, this is the first time ever to disclose the exact parameters defining the three-dimensional structure of a protein component of the leukotriene cascade. Due to these novel reliable parameters, the complex as well as the components thereof are readily distinguished from the prior art. Together with biochemical and mutagenetic data, the novel structures will provide the basis for understanding the molecular mechanisms of the aminopeptidase and epoxide hydrolase activities, as well as the enzyme's suicide inhibition. Accordingly, the present invention will open a whole range of new possibilities as regards e.g. identification and/or design of novel biologically active molecules and methods of controlling said cascade, *in vivo* or *in vitro*. Consequently, novel advantageous drugs, such as medicaments for the treatment and/or prevention of inflammatory and/or allergic diseases, may be designed, as will be discussed in further detail below.

In the present context, it is to be understood that proteins according to the invention include the naturally occurring three dimensional forms thereof, separated and isolated from its natural environments, as well as any such protein, wherein deletions, additions and/or substitutions of the amino acid sequence have been made, provided that the three dimensional structure is substantially maintained, as the exerted biological activity is critically dependent upon the particular three-dimensional folding of the protein. The present invention also encompasses any derivative or conformational analogue of the above disclosed proteins, which has a three-dimensional structure essentially as disclosed above, or an effective part thereof having the biological activities discussed in detail below.

25

30

5

2.4.4 Advantageous uses of LTA₄ hydrolase, complementary compounds and complexes thereof

A fourth aspect of the present invention is the use of a protein, a complementary compound or a complex according to to the invention in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry. Such methods will be disclosed in detail below. The drugs designed using the above mentioned compounds may be suitable for the treatment and/or prevention of disorders involving acute and chronic inflammatory symtoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS). Further, such a drug may be useed for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer. Alternatively, a drug may be designed which is effective for the treatment and/or prevention of an inflammatory and/or allergic disorders caused by the lethal factor of Bacillus anthracis, e.g. anthrax. However, the above mentioned diseases are exemplary and other diseases or conditions not mentioned herein may also be contemplated.

In a further aspect, the present invention relates to the use of a protein having a structure substantially as defined for the LTA₄ hydrolase of the invention, or a part, analogue or derivative thereof, for screening a compound for possible medicinal activity. In the pharmaceutical industry, new or known compounds are routinely screened for new uses employing a variety of known *in vitro* or *in vivo* screens. Often such screens involve complex natural substances and are consequently expensive to carry out, and the results may be difficult to interpret. However, the knowledge of the three-dimensional protein structure according to the invention allows a preliminary screening to be carried out on the basis of the three-dimensional structure of a region thereof, and the structural similarity of a molecule which is being screened. Such screening can conveniently be carried out using computer modelling techniques, which match the three-dimensional structure of the protein or part thereof with the structure of the molecule being screened. Potential agonist or inhibitor activity may be predicted. As a result, the production efficiency, bioavail-

10 and the state of the state o

5

ability, immunogenicity, stability etc. may be favourably changed with respect to their therapeutic application.

As regards the above disclosed M1 inhibitors, these compounds will presumably find a broader field of application than the other novel inhibitors according to the invention. Thus, the novel general M1 inhibitors are advantageously used e.g. in models to disclose in further detail other enzymatic pathways. Further, they may also be used in the above mentioned type of methods of drug design etc.

2.4.5 Screening for LTA₄ hydrolase analogues

2.4.5 (a) Method

Accordingly, in another aspect, the invention relates to a method for screening LTA₄ hydrolase analogues that mimic at least a part of the three dimensional structure of LTA₄ hydrolase, which comprises the steps of

- (a) producing a multiplicity of analogue structures of the LTA₄ hydrolase
- (b) selecting an analogue structure represented by a three-dimensional representation wherein the three-dimensional configuration and spatial arrangement of specific regions, preferably involved in ligand binding of said LTA₄ hydrolase, remain substantially preserved.

The coordinates used are general for LTA₄ hydrolase are essentially as illustrated in Table 9, as defined by atom nos. 1-4876.

More specifically, analogue structures of LTA4 hydrolase may be screened by their ability to catalyze a particular reaction which may be monitored by chemical physical or immunological means. Furthermore, the analogue structure may be selected from its ability to produce receptor ligands or inhibitors of secondary reactions, which may be monitored directly, as examplified above, via binding assays, enzyme assays, chemical assays, or functional bioassays.

Thus, in one embodiment, the invention relates to a method of screening, wherein one or more analogues exhibiting epoxide hydrolase activity, are screened for. Thus, such a method may be based on the data of Table 9, wherein the binding of thiolamine to LTA₄ hydrolase is shown, preferably combined with the information of Table 3 regarding the active site of LTA₄ hydrolase. In one embodiment, the

25

30

10

15

20

25

invention relates to a method of screening, wherein one or more analogues exhibiting epoxide hydrolase activity, are screened for. In an alternative embodiment, the present method is used to screen for analogues exhibiting aminopeptidase activity, which method e.g. is based data concerning the binding of bestatin to LTA₄ hydrolase is used, preferably combined with the information of Table 2 regarding the active site of LTA₄ hydrolase. Thus, the present analogues will comprise a region which is essentially analogue with the regions of LTA₄ hydrolase exhibiting aminopeptidase activity, and/or analogues exhibiting epoxide hydrolase activity are selected.

In an advantageous embodiment of the screening method according to the invention, one or more analogues comprising one or more genetic modifications, as compared to the naturally occurring form of LTA₄ hydrolase, are selected.

2.4.5 (b) Analogues obtainable by the present screening method

Further, the invention also relates to a novel analogue obtainable by the method according to the invention, such as an analogue exhibiting an increased or improved or otherwise modified catalytic activity when compared to the naturally occurring form of LTA₄ hydrolase. Preferably, said catalytic activity is an epoxide hydrolase and/or aminopeptidase activity. Further, the invention relates to an analogue obtainable by the present method and capable of acting as a metallohydrolase, preferably belonging to the M1 class of metallohydrolases.

2.4.5 (c) Mutated forms of LTA₄ hydrolase obtainable by the present screening method

In one advantageous embodiment, the present invention relates to a specified analogue which is a mutated form of LTA₄ hydrolase, which analogue comprises one or more of the mutations defined in the following Tables 5-7, wherein amino acids are given in single letter code. Thus,

Q134G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W indicates that residue glutamine 134, using the LTA4 hydrolase numbering scheme, is modified to an alanine, valine, a leucine and so forth.

40

Table 5: Mutations in the active site

	Q134G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W	5(1)
	Q136G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W	5(2)
5	A137G/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(3)
	Y267G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W	5(4)
	G268A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(5)
	G269A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	56)
	M270G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/F/Y/W	5(7)
10	E271G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	5(8)
	V292G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(9)
	H295/G/A/V/L/I/S/T/D/E/N/Q/R/K/P/C/M/F/Y/W	5(10)
	E296/G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	5(11)
	H299G/A/V/L/I/S/T/D/E/N/Q/R/K/P/C/M/F/Y/W	5(12)
15	W311G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y	5(13)
1=0	F314G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/Y/W	5(14)
## ·	W315G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y	5(15)
in Li	E318G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	5(16)
þ.k.	V322G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(17)
20	F362G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/Y/W	5(18)
	V367G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(19)
	L369G/A/V/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(20)
# # # # # # # # # # # # # # # # # # #	1372G/A/V/L/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(21)
	P374G/A/V/L/I/S/T/D/E/N/Q/R/H/K/C/M/F/Y/W	5(22)
25	D375G/A/V/L/I/S/T/E/N/Q/R/H/K/P/C/M/F/Y/W	5(23)
	A377G/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(24)
	Y378G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W	5(25)
	P382G/A/V/L/I/S/T/D/E/N/Q/R/H/K/C/M/F/Y/W	5(26)
	Y383G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W	5(27)
30	R563G/A/V/L/I/S/T/D/E/N/Q/H/K/P/C/M/F/Y/W	5(28)
	<u>-</u>	()

More specifically, this embodiment relates to an analogue comprising any combination of at least two mutated amino acids, or any one of the above mentioned sequences of mutations, or any separate one amino acid mutation selected from the group consisting of sequences nos 1-9, 13-15, 17-24, 26 and 28, which are all novel mutations that have never been published before the present application. As two specific embodiments of the present mutations according to the invention, E271Q and D375N are mentioned, which have shown to be especially advantageous. However, the other sequences not specified above are novel in the present context and thus such specific uses thereof are within the scope of the present invention.

	Table 6: Mutations of the curved outside o	f the N-terminal domain
	R17 G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W	6(1)
	K19 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(2)
	H20 G/A/V/L/I/S/T/D/N/E/Q/R/K/P/C/M/F/Y/W	6(3)
5	H22 G/A/V/L/I/S/T/D/N/E/Q/R/K/P/C/M/F/Y/W	6(4)
	R24 G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W	6(5)
	D28 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	6(6)
	T33 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(7)
	T35 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(8)
10	G36/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(9)
	T37 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(10)
	A39 G/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(11)
	T41 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(12)
	Q43 G/A/V/L/I/S/T/D/N/E/R/H/K/P/C/M/F/Y/W	6(13)
15	K63 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(14)
43	V65 G/A/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	• •
	N67 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W	6(15)
25 miles	N97 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W	6(16)
<u>L</u>	E99 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(17)
²⁶ 20	V101 G/A/L/JS/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(18)
#	E103 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(19)
h Nj	\$105 G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(20)
T.	E107 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(21)
	K153 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(22)
25	T155 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(23)
- 2J	T157 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(24)
	E159 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(25)
	S161 G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(26)
	D175 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	6(27)
30	E177 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(28)
	T178 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(29)
	D180 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	6(30)
	R186 G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W	6(31)
	1188 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(32)
35	K190 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(33)
	1192 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(34)
	K194 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(35)
	MIDT GITE VILLES INDINIE QINHIP CIMIFI YIW	6(36)
	Table 7: Mutations at the proline	e rich region
40	T359 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(1)
	E358 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	7(2)
	D443 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	7(3)
	A446 G/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(4)
	Y449 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/W	7(5)
45	S450 G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(6)

	^
- 1	0
-	. •
.622.227	
124	
400	
in the	
ja A.	
1	_
3700	. 3
1 m	
\$ 2000 1600 EDIO	
UT	
52 3	
]= £.	
State Season	
華	
R c	
k.	
FF 3	
M.	
T.	
44	
	Ω
112	U
AT ALL	
11	

30

5

	P451 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(7)
	G452 /A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(8)
	L453 G/A/V/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(9)
	P454 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(10)
	P455 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(11)
	I456 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(12)
	K457 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	7(13)
	P458 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(14)
	N459 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W	7(15)
)	Y460 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/W	7(16)
	D461 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	7(17)

2.4.5 (d) Nucleic acids encoding the novel compounds

Further, the invention also relates to an isolated nucleic acid encoding a novel analogue as defined above, that is, including a combination of any at least two of said mutations or one of the novel mutations, as well as a nucleic acid capable of specifically hybridising to a such a nucleic acid. The conditions of specific hybridisation are defined above in the section "Definitions". Further, the invention also relates to any vector or carrier comprising such a nucleotide, such as plasmids, viral vectors, e.g. retrovirus, oligonucleotides etc. Thus, any cell including such a nucleic acid or vector are also within the scope of the present invention and may e.g. be a mammalian cell, such as a human cell, or any other eucaryotic cell, or a procaryotic cell, such as a bacterium. The above mentioned elements may be used in the design of model systems useful in the study of the diseases discussed elsewhere in this application, which systems may be cell cultures, animal models, such as mice, etc.

2.4.6 (a) Production and purification of genetically modified forms of LTA₄ hydrolase

Yet another aspect of the present invention is a process for the production of a novel genetically modified form of LTA₄ hydrolase identified or designed according to the present invention. Thus, the present process involves, after conventional steps of insertion a gene encoding the desired product in a host cell and expression thereof, a purification procedure, which includes a hydroxyapatite-based chromatography and a subsequent anion exchange chromatography. These last two steps have been shown to be especially advantageous, in fact, even crucial, for obtaining a

5

satisfying purity of the novel LTA₄ hydrolase forms according to the invention. The preceding steps are conventional as disclosed in literature and are easily performed by the skilled in this field.

Thus, in more detail, the invention relates to a method for purification of LTA4 hydrolase comprised of (i) precipitation with ammonium sulphate, followed by (ii) separations on FPLC using anion exchange, hydrophobic interaction, and chromatofocusing resins, essentially as described (Wetterholm A., Medina J.F., Rådmark O., Shapiro R., Haeggström J.Z., Vallee B.L., Samuelsson B. *Biochim. Biophys. Acta.* 1080, 96-102 (1991)). To achieve a purity suitable for crystallography, we used (iii) chromatography on hydroxyapatite, e.g., on a TSKgel HA-1000, Tosohaas, followed by (iv) a step of anion-exchange chromatography on e.g., Mono-Q HR5/5.

Further, example 4 below describes in detail a purification of LTA₄ hydrolase according to the invention. Said example may be generalised to describe further the purification according to the invention.

2.4.6 (b) Purified LTA₄ hydrolase

Further, the invention also relates to an essentially pure form of LTA₄ hydrolase obtained by the process described above.

2.4.7 Identification of LTA₄ hydrolase binding compounds

2.4.7 (a) Method

In yet a further aspect, the present invention relates to a method for screening LTA₄ hydrolase binding compounds complementary to a region, preferably an enzymatically active site, e.g. as defined in Tables 1-3, of the LTA₄ hydrolase molecule, which comprises the steps of

- (a) producing a multiplicity of possible complementary structures and
- 25 (b) selecting a structure represented by a three-dimensional representation, wherein the three-dimensional configuration and spatial arrangement of regions of LTA₄ hydrolase involved in binding remain substantially preserved, which selection is based on the three-dimensional structure of LTA₄ hydrolase and/or LTA₄ hydrolase complexed to an inhibitor thereof, e.g. as defined by the coordinates of Table

25

30

5

More specifically, the method according to the invention will advantageously be used to select compounds capable of inhibiting epoxide hydrolase activity and/or aminopeptidase activity, LTB₄ receptor antagonists or inhibitors of LTC₄ synthases or inhibitors of any member of the M1 class of metallohydrolases. In one preferred embodiment, general enzyme inhibitors are screened for, which inhibitors are useful in the control of any one of a plurality of enzymatic pathways, wherein a metallohydrolase of the M1 type is participating. These general metallohydrolase inhibitors are herein denoted M1 inhibitors.

Structure-based design of inhibitors

In a further embodiment, the present invention relates to a method of structure-based design of LTA₄ hydrolase inhibitors. Such methods are based on the use of the present coordinates, or preferably the coordinates defining a selected region, as templates in order to synthesize advantageous inhibitors with strong and specific binding properties. More specifically, said method first uses a conventional organic synthesis, alone or combined with combinatorial chemistry, wherein the structure of the product of the synthesis is then further refined by cycles of crystallisation of enzyme and inhibitor, followed by another chemical synthesis, the product of which is again refined, etc.

Example 2 describes such a design, wherein it is noted noted that the removal of an extra carbon atom could yield a compound, which is a better inhibitor than this hydroxamic acid compound. Thus, similar conclusions will be drawn from the present method and result in inhibitors with superior properties compared to any prior art inhibitors.

2.4.7 (b) Identified binding compounds

Further, the present invention also relates to any novel compounds identifiable by the present method. Advantageous and desired properties as well as other features of such compounds, e.g. as inhibitors, is discussed above in relation to complementary compounds, analogues etc. In one preferred embodiment of the invention, such an identified compound is an inhibitor of another M1 enzyme than LTA₄ hydrolase, such as . The medicinal aspects of the present compounds will be discussed below.

Protein engineering

2.4.8 (a) Method

In a further aspect, the present invention relates to a method of engineering a protein, which method comprises the steps of

- -identification of a suitable set of mutation sites based on the structure of LTA₄ hydrolase according to the invention,
- -generation of a library of genes which contains the suitable sequence variations;
- -selection of clones encoding a LTA4 analogue with a desired activity;

wherein said desired activity is the capability of efficiently producing organic compounds of interest.

The present method is based on recent techniques available for generating large libraries of mutated genes (>1 billion variants) which can be attributed to a selection process of individual genes in the laboratory. Such directed evolution schemes have enormous potential for the design of new proteins, including new substrate specificity for enzymes as well as improving enzyme activities.

Directed evolution, or combinatorial engineering schemes have been successfully applied in evolving RNA molecules with improved binding and catalytic activities (Lorsch and Szostak, 1994). Also binding proteins (and peptides) with good affinities can now routinely be evolved based on a range of different protein folds (Nord et al, 1997). The present methods may be used to perform such a directed evolution of advantageous enzyme activity and specificity and may be performed by someone skilled in this field with reference to the literature, see e.g. O. Kuchner and F. H. Arnold (1997); A. Crameri, S.A. Raillard, E. Bermudez and W.P.C.

Stemmer (1998).) In this context, see also the descriptions provided in US patent no 5 873 082, Noguchi, wherein a list processing system for managing and processing lists of data is disclosed; US patent no 5 869 295, LaBean et al., disclosing methods and materials for producing gene libraries; and US patent no 5 856 928, disclosing a process for gene and protein representation, characterization and interpretation thereof.

In general, major difficulties in this kind of process are to search the sequence space: find the suitable sequence variations for a large but limited number of muta-

30

25

25

5

tions (for the same protein fold an immense number of variations can be made e.g. 10 resides protein, 20^{100} variants are in theory possible). It is therefor very important to identify the residues in the protein structure which could effect the activity the most, i.e. the residues near the active site area. Thus, in order to enable a successful performance of a method for engineering proteins with properties relevant in the present field, the data discosed above, more specifically, in Tables 2-4, is crucial.

Further references which are relevent in the context of protein engineering are K. Nord, E. Gunneriusson, J. Ringdahl, S. Stahl, M. Uhlen, P.A. Nygren (1997): "Binding proteins selected from combinatorial libraries of an alpha-helical bacterial receptor domain", *Nature Biotechnology*, 15, 772-777 (1997); R. Lorsch and J.W. Szostak (1994): "In vitro evolution of new ribozymes with polynucleotide kinase activity", *Nature*, 371, 31-36; A. Crameri, S.A. Raillard, E. Bermudez and W.P.C. Stemmer (1998): "DNA shuffling of a family of genes from diverse species accelerates directed evolution", *Nature*, 391, 288-291; and O. Kuchner and F. H. Arnold (1997): "Directed evolution of enzyme catalysts", *Trends in Biotechnology*, 15, 523-530.

In an advantageous embodiment, the present method is used to engineer LTA₄ hydrolase inhibitors and/or analogues. In a specific embodiment of said method, a compound capable of mimicking the suicidal mode of LTA₄ hydrolase catalysis, thus acting as a mechanism-based suicide inhibitor, or otherwise capable of regulating the production of LTB₄ is engineered. In an alternative embodiment, an inhibitor of LTC₄ synthase or an LTB₄ receptor antagonist is designed.

2.4.8 (b) Novel specifically designed proteins

Further, the present invention also relates to any novel protein designed by use of the above described method. Once specified, such proteins may be produced by any conventional method well known to the skilled in this field, some of which are examplified below. In Example 2 below, the binding of hydroxamic acid to LTA4 hydrolase is discussed. Thus, such a modified hydroxamic is one example of a novel inhibitor specifically designed according to the invention, and the resoning in the

5

example may be used as a basis for the way of reasoning that is used in the present design.

Accordingly, novel enzymes may be produced, which are capable of any different chemical activity. For example, enzymes capable of novel catalytic properties, enzymes that in turn produce enzymes, etc., may be produced according to the present invention.

2.4.8 (c) Use of genetically modified LTA₄ hydrolase

The invention also encompasses the use of a genetically modified LTA4 hydrolase, obtained by any method according to the invention, with altered catalytic properties, e.g., increased ability to synthesize LTB4. The modified enzyme may thus be used for production of LTB4, or any analogues substances, a biomedical reagent which in turn may be used in, e.g., studies of leukotriene metabolism, induction of chemotaxis, as a reference compound in analysis of leukotrienes etc.

2.4.9 Pharmaceutical applications of the present invention

2.4.9 (a) First medical indication

Further, the invention also encompasses a compound obtainable by the method of screening LTA₄ hydrolase binding compounds, structure-based drug design, or the protein engineering methods described above, and more preferably, said compound for use as a medicament. One specifically advantageous embodiment is the herein disclosed novel M1 inhibitor for use as a medicament.

In an advantageous embodiment, the present compounds are used in the manufacture of a medicament for the treatment and/or prevention of acute and chronic inflammatory disorders, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis and chronic obstructive pulmonary disease (COPD); neoplasias and/or cancer; or disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax. Alternatively, the use may relate to the manufacture of a medicament for the treatment and/or prevention of an inflammatory and/or allergenic disorder, such as bronchial asthma, allergic rhinitis, conjunctivitis etc. Yet an alternative use is in the manufacture of a medicament for the treatment and/or prevention of infection caused be human immunodeficiency virus

25

30

5

(HIV). The novel M1 inhibitor are preferably used in medicaments for the treatment and/or prevention of such various diseases as cancer and/or endochrinological disturbances.

2.4.9 (b) Second medical indication and pharmaceutical methods

Thus, the present invention relates to the above mentioned molecules prepared by the method according to the invention for use in the manufacture of various medicaments for the above defined conditions. The invention also encompasses pharmaceutical preparations containing these molecules together with pharmaceutically acceptable carriers. Methods for the preparation of pharmaceutical preparations are e.g. found in Remington's Pharmaceutical Sciences, Mack Publishing Company, Philadelphia, PA, 17th ed. (1985). For a review of drug delivery, see Langer, Science 249:1527-1533 (1990). As those skilled in this field easily realise, the form of such a pharmaceutical preparation, the mode of administration thereof as well as suitable dosages will depend on the specific disease to be treated, the nature of the active substance used, the patient's age, body weight etc.

2.4.9 c) Methods of treatment

The present invention also encompasses any method of treatment for the above defined purposes. Exact details regarding such methods are determined by the practitioner depending on the specific circumstances from case to case.

2.5 Production of novel proteinaeous compounds

The compounds, which may be proteins, polypeptides, peptides or any other organic molecules, prepared according to the methods according to the invention may be synthesized chemically by methods well known to those of skill in this field or they may be prepared by use of recombinant DNA technology by any suitable method well known to those of skill in this field. General methods of synthesis are e.g. found in Berger and Kimmel, Guide to Molecular Cloning Techniques, Methods in Enzymology, vol. 152, Academic Press, Inc., San Diego, CA; Sambrook et al., Molecular Cloning, A Laboratory Manual, 2nd Ed., vol. 1-3, Cold Spring Harbor Laboratory, Cold Spring Harbor, NY, 1989; and Current Protocols in Molecular Biology, F.M. Ausbel et al., Current Protocols (1994). Methods of reducing and denaturing proteins and inducing re-folding are well known to those of skill in the art,

15

20

30

see e.g. Debinski et al., J. Biol. Chem., 268: 14065-14070 (1993); Kreitman and Pastan, Bioconjug. Chem., 4: 581-585 (1993); and Buchner et al., Anal. Biochem., 205: 263-270 (1992).

2. 6 Detailed description of the drawings

5 Figure 1 shows key enzymes and intermediates in leukotriene biosynthesis.

Figure 2 shows 2Fo-Fc density contoured at 1.1 σ. Part of the active site in the neighborhood of the bestatin molecules is shown. Figures are created using a modified version of Molscript48,49.

Figure 3 is a ribbon diagram of the tertiary structure of LTA4 hydrolase. The N-terminal domain at the top of the diagram is rich in β -strands and connects to the catalytic domain to the left in the figure which is more α -helical and extends into the central part of the molecule. The C-terminal domain, illustrated at the bottom of the ribbon diagram, extends towards the right side of the catalytic domain.

Figure 4 (a) is a ribbon diagram of the N-terminal domain with its layers of β -strands, while (b) is a superimposition of the C α trace of the N-terminal domain on the C α trace of bacteriochlorophyll a. The N-terminal domain covers approx. half of the bacteriochlorophyll a structure (the right and bottom part of the diagram).

Figure 5 (a) is a ribbon diagram of the catalytic domain. In the center of the diagram, the three zinc binding ligands, His295, His299, and Glu318, as well as the inhibitor bestatin are depicted in ball and stick representation. The zinc ion is shown as a CPK model. The diagram in (b) shows the structure of thermolysin in the same orientation as the catalytic domain of LTA4 hydrolase. The three zinc ligands, His142, His146, and Glu166, as well as the inhibitor Cbz-GlyP-(O)-Leu-Leu50 are depicted in ball-and stick representation. The zinc ion is shown as a CPK model.

Figure 6 shows the structure of the C-terminal domain.

Figure 7 shows the zinc binding ligands in LTA4 hydrolase, His295, His299, and Glu318, superimposed on those in thermolysin, His142, His146, and Glu-166. Other catalytic or neighboring residues in the two enzymes are Tyr383, Glu325, Glu296, Thr302, and Asn317 in LTA4 hydrolase which correspond to His231, Asp170, Glu143, Asn165, and Tyr157 in thermolysin.

25

5

Figure 8 (a) is a Ball-and-Stick presentation of the binding of bestatin in LTA4 hydrolase.

Figure 8 (b) is a schematic overview of bestatin binding in LTA4 hydrolase.

Figure 9 (a) is a wire representation of the cavity found in LTA4 hydrolase (shown as $C\alpha$ -trace).

Figure 9 (b) is a schematic presentation for the proposed binding of LTA4 into the cavity.

Figure 10 is a schematic representation for the proposed epoxide hydrolase reaction mechanism. The catalytic zinc acts as a Lewis acid and activates the epoxide to form a carbocation intermediate according to an SN1 reaction. Water is added at C12 in a stereospecific manner, presumably directed by Asp375. The double bond geometry is controlled by the binding conformation of LTA4. Further details are given elsewhere in the present description.

3. EXPERIMENTAL

The following examples are intended for illustrating purposes only and should not in any way be used to construe the scope of the protection of the present invention as defined by the appended claims. All the references given below, and previously in this specification, are hereby included herein by reference.

3.1 Examples

Example 1: Binding of the thiol-compound (I)

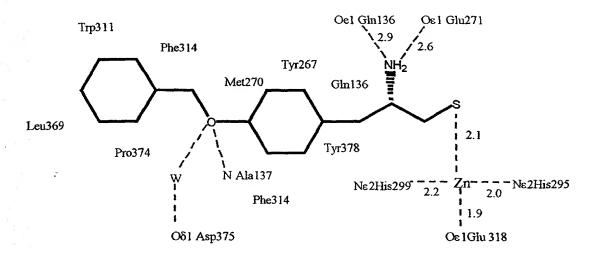
The thiol group of the compound is ligated to the Zn²⁺ ion, that has a tetra-hedral configuration. Both the phenyl-groups are making extensive hydrophobic interactions. The first one makes aromatic stacking interactions with Phe314 and Trp311. Further hydrophobic interactions are made with Pro374 and Leu369. The other phenyl ring is making stacking interactions with Tyr267 and Tyr378. Met270 and Gln136 provide additional hydrophobic interactions. The ether-oxygen in the linker between the two phenyl rings makes a hydrogen bond to the backbone nitrogen of

10

15

20

Ala137 and also with a water molecule which is linked to Asp375. The amine group makes interactions to the Oɛ1 of Gln136 and the Oɛ1 of Glu271.



Formula (I)

Example 2: Binding of the hydroxamic acid compound (II)

The binding of this compound is very similar to the binding of the thiol compound described above. The manner in which the phenyl-moieties, the linker region and the amine group are bound is identical. The manner in which the hydroxamic acid part is bound is different in comparison with other complexes such as thermolysin-HA complexes and LTA₄-hydrolase-bestatin complex. Instead of a double interaction of the hydroxyl and carbonyl oxygens and the Zn ion resulting in a pentavalent co-ordination, here only one of the oxygens (the hydroxyl) is making an interaction with the Zn ion giving a tetrahedral co-ordination. The other oxygens make an interaction to Asp296 and the backbone nitrogen of Gly268. This difference is probably due to the tight binding of the phenyl rings and the amine group. The linkage between the amine group and the hydroxamic acid group contains one more carbon atom than in a normal or modified peptide-linkage. Since the binding site for substrates is rather narrow near the Zn ion, the conformation of compounds which bind in this area is rather restricted. Therefore one of the otherwise binding oxygens is pushed out and can no longer make an interaction with the Zn²⁺ ion. Removal of this extra

20

carbon atom could yield a compound which is a better inhibitor than this hydroxamic acid compound. The acid group at the other end of the compound is fixed by making a double interaction with the Ne and the Nh2 of Arg563.

Formula (II)

Example 3: Structure determination of two specific inhibitor-LTA₄ hydrolase complexes

Crystals, grown as described above, were soaked in 1 mM solution of thiolamine (Yuan et al., 1993) or 0.5 mM solution of hydroxamic acid (Hogg et al., 1995) in 15% PEG8000, 50 mM Imidazol pH 6.7, 25 mM acetate and 2.5 mM YbCl3. After at least 24 hours, the crystals were transferred to a solution that contained a cryoprotectant (see above) and subsequently flash frozen in liquid nitrogen. The data for the crystal soaked with thiolamine was obtained at BM14B at the EMBL-outstation in DESY, Hamburg. The data for the hydroxamic acid was collected at beamline 7/11 at MAX-lab, Lund. Statistics from the data collections are shown in the table. The data were processed using MOSFLM, merging and other manipulations were performed by programs from CCP4 and the BIOMOL packages. The refinement procedures for both datasets were very similar. First rigid body refinement using TNT was performed. As a starting model for refinement and model building the structure of LTA4 hydrolase complexed with bestatin was used. The bestatin molecule and all water molecules were deleted from the model. After this initial refine-

10

15

20

ment it was possible to build the inhibitors into the protein. For evaluation of the density maps and model-building the program QUANTA (Molecular Simulations Inc., Burlington, MA) was used. The refinement was continued using TNT and was combined with sessions of model-building. In all rounds no sigma cut-offs were used and the resolution was slowly increased during the procedure. Water molecules were identified and incorporated into the models. During these procedures the Rfree was carefully monitored. When refinement had converged, it was finished with one round in which all reflections, including those who were used for the calculations of the Rfree, were incorporated. Statistics about refinement and quality of the models can be found in Table 5.

Table 8: Statistics of refinement and quality of the model

	Thiolamine (Thiol)	Hydroxamic acid (HA)
Resolution	15-2.5Å	15-1.8Å
Rfactor	17.8%	24.2%
Rfree	24,4	29.7%
Bond Lengths	0.011Å	0.012Å
Angles	1.9°	2.0°
Trigonal groups	0.005Å	0.006Å
Planar groups	0.009Å	0.010Å
Contacts	0.026Å	0.041Å
No. of waters	252	127

Example 4: Purification of LTA4 hydrolase.

For adsorption chromatography on hydroxyapatite, a TSKgel HA-1000 column (Tosohaas) was equilibrated in 10 mM potassium phosphate buffer, pH 7.1, supplemented with 0.2 mM CaCl₂. The enzyme sample was applied and a linear gradient of increasing phosphate (10 - 400 mM) was developed by mixing the starting buffer with 400 mM potassium phosphate buffer, pH 6.8, supplemented with 10 µM CaCl₂. Active fractions containing LTA4 hydrolase were eluted between 150 - 190 mM potassium phosphate.

5

Anion exchange chromatography was performed on a Mono-Q HR 5/5 column (Pharmacia Biotech) equilibrated with the loading buffer 10 mM Tris-Cl, pH 8. The pure protein was eluted using a linear gradient of KCl (0 - 500 mM) and was recovered at 110 - 140 mM KCl.

Example 5: Enzyme engineering

The present inventors have shown, that when Tyr-378 in LTA4 hydrolase was exchanged for a Phe residue, the resulting mutated enzyme was no longer suicide inhibited by LTA4 and exhibited a substantially increased catalytic efficiency. Furthermore, the mutated enzyme was capable of converting LTA4 not only into the natural product LTB4, but also into a novel metabolite, 6-trans-8-cis-LTB4. (Mueller, M.J., et al. Proc Natl Acad Sci U S A 93, 5931-5935 (1996)).

Example 6: Enzyme-engineering

Tyr-383 in mouse LTA4 hydrolase was exchanged for Gln residue, which resulted in a mutated enzyme capable of forming the unnatural product 5S, 6S-dihydroxy-7,9-trans-11,14-cis-eicosatetraenoic acid from LTA4 (Andberg, M., Hamberg, M. & Haeggstrom, J.Z. J. Biol. Chem. 272, 23057-23063 (1997)).

Example 7: Crystallisation of LTA₄ hydrolase

LTA₄ hydrolase was crystallised using YbCl₃ as an additive, 15% PEG and 50 mM Na-acetate as precipitant and 50 mM imidazole, pH 6.7, as buffer. Liquid-liquid-diffusion in capillaries were used as crystallisation set-ups.

3.2 Materials and Methods

Enzyme purification. Human recombinant LTA4 hydrolase was expressed in E. coli and purified to homogeneity in four chromatographic steps on FPLC using anion exchange, hydrophobic interaction, chromatofocusing, and hydroxyapatite resins, essentially as described (Wetterholm A., Medina J.F., Rådmark O., Shapiro R., Haeggström J.Z., Vallee B.L., Samuelsson B. Recombinant mouse leukotriene A4 hyd-

20

25

5

rolase: a zinc metalloenzyme with dual enzymatic activities. *Biochim. Biophys. Acta.* 1080, 96-102 (1991)).

Crystallization conditions. The chemicals used for the crystallization experiments were purchased from Merck and were of highest purity available. The sparse matrix kit was obtained from Hampton Research. Crystallization conditions for the protein were initially sought by using the sparse matrix approach (Jancarik, J. & Kim, S.-H. J. Appl. Crystallogr. 24, 409-411 (1991)) in hanging drop vapor diffusion set-ups in cell culture plates at room temperature. Under condition 28, (30% PEG8000, 0.2 M sodium-acetate, 0.1 M cacodylate buffer, pH 6.5) needles grew. They were subsequently reproduced and optimized using a finer grid search, different temperatures for the equilibration and testing of additives. Crystals were only obtained when the inhibitor bestatin was present in the crystallization set-ups. Using YbCl3 as an additive and switching to liquid-liquid diffusion in capillaries, allowed plate-like crystals to grow. Thus, 5 µl 28% PEG8000, 0.1 mM Na-acetate, 0.1 mM imidazole buffer, pH 6.8, 5 mM YbCl3 is injected into the bottom of a melting point capillary and an equal volume of LTA4 hydrolase (5 mg/ml) in 10 mM Tris-Cl, pH 8, supplemented with 1 mM bestatin, is layered on top. Finally, the capillary is closed and stored at 22°C. Crystals with an average size of 0.6 x 0.4 x 0.05 mm³ appear in 3 to 4 weeks.

<u>Crystal properties</u>. The plate-like crystals diffract beyond 2Å using synchrotron radiation. They belong to space-group P21212 with cell dimensions a = 67.59 Å, b = 133.51 Å, c = 83.40 Å, $a = b = g = 90 ^{\circ}$ at 100K. As a cryo-solution, a mixture of 15%PEG 8000, 50 mM Na-acetate, 50 mM imidazole buffer, pH 6.8, 2.5 mM YbCl3, and 25% glycerol was used. Assuming one molecule per asymmetric unit the solvent content of the crystals is 48%.

Structure determination. The structure was determined by using multiple anomalous dispersion measurements on the LIII edge of Ytterbium ($\lambda = 1.3862$ Å) at beam line BM14 at the European Synchrotron Radiation Facility (ESRF), Grenoble. Three datasets, peak (PK), point of inflection (PI) and remote (RM), were collected to 2.5Å resolution from the same crystal. The crystal was aligned such that Bijvoet

25

30

5

equivalent reflections could be collected in one pass of 90° for each wavelength. For RM a subsequent dataset to 2.15Å was collected. A second crystal was used for obtaining a dataset to 1.95Å. (For statistics on data-collection and quality, see table 1). Data were integrated using the program Denzo, scaled to each other using Scalepack (Otwinowski, Z. Data collection and Processing. Proceedings of the ccp4 study weekend. SERC Daresbury Laboratory, Warrington, UK., 56-62 (1993)) and further analyzed using programs from the CCP4 package (Collaborative Computing Project Number 4. Acta Crystallogr. Sect. D 50, 760-763 (1994)).

From Patterson functions one major and one minor Yb position could readily be identified, a third position was identified during heavy atom refinement in difference Fourier maps. The heavy atom parameters were refined using MLPHARE (Otwinowski, Z. Isomorphous replacement anomalous scattering. Proceedings of the CCP4 study weekend. SERC Daresbury Laboratory, Warrington, UK., 80-85 (1991)) and SHARP (de La Fortelle, E. & Bricogne, G. Met. Enzymol. 276, 472-494 (1997)). The final figures of merit was 0.57 to 2.15Å. Phase information was further improved to 2.15Å by solvent flattening using SOLOMON (Abrahams, J.P. & Leslie, A.G.W. Acta Crystallographica D52, 30-42 (1996)) with a solvent content of 43%. The quality of the maps was very good and the entire protein molecule (residue 1-610) could be traced unambiguously. All model building was performed using QUANTA (Molecular simulations). Refinement was started by a run of slowcooling molecular dynamics in XPLOR (Brünger, A.T., Kuriyan, J. & Karplus, M. Science 235, 458-460 (1987)) using the RM dataset to 2.7Å. The three Yb ions were included into the refinement with full occupancy for the first Yb and half occupancy for the two other ions. All subsequent refinement was performed with TNT (Tronrud, D.E., ten Eyk, L.F. & Matthews, B.W. Acta Crystallogr. Sect. A 43, 481-501 (1987)). The same set of reflections (4% of total amount from 25-1.95Å) for the calculation of Rfee (Brünger, A.T. Nature 355, 472-475 (1992)) was maintained throughout all refinement procedures. The resolution was slowly improved by alternating sessions of model-building and refinement. The data for the second crystal to 1.95Å were used for further refinement during which a Zn ion, bestatin, an acetate

10

15

20

and an imidazole molecule were identified. Judged from the B-factors these molecules are all fully occupied. 540 water molecules were added to the coordinates. The Rfree was 24.7% and the working R-factor was 18.8% for all data between 25-1.95 Å. In a final round of refinement all data between 25-1.95 Å were included, yielding a final R-factor of 18.5 % for residues 1-610, 3 Yb ions, 1 Zn, 1 bestatin, 1 imidazole, 1 acetate and 540 water molecules. Most of the model is in good density (Fig. 2) except a loop encompassing residues 179 to 184 for which only poor density was obtained. The model has good stereo-chemical parameters (r.m.s bonds =0.010Å, r.m.s angles = 2.2°) and 91.7% of the residues lie in the most favored part of the Ramachandran plot.

4. RESULTS AND DISCUSSION

4.1 Overall structure and domain organization

The leukotriene A4 hydrolase molecule is folded into three domains; an N-terminal domain, a catalytic domain and a C-terminal domain which together form a flat triangular arrangement with approximate dimensions of $85 \times 65 \times 50 \text{ Å}^3$. The overall structure of the enzyme is depicted in figure 3. Although the three domains pack closely and make contact with each other, a deep cleft is formed in between.

4.2 The N-terminal domain is structurally related to bacteriochlorophyll a

The N-terminal domain (residue 1-209) is composed of one 7 stranded mixed b-sheet, one 4 and one 3 stranded antiparallel β -sheet. Strands from the larger β -sheet continue into the two smaller β -sheets that pack on the edges of the same side of the larger sheet so that a kind of envelope is formed (Fig. 4a & b). The two small β -sheets are turned towards the inside of the whole protein while the larger β -sheet is exposed to solvent and forms a large concave surface area. Loops connecting the other strands and hydrophobic residues fill the core of this domain. The N-terminal domain of LTA4 hydrolase shares important structural features with the chlorophyll-containing enzyme bacteriochlorophyll (Bchl) α (Matthews, B., Fenna, R., Bolognesi, M., Schmid, M. & Olson, J. J. Mol. Biol. 131, 259-285 (1979)). Thus, 111 C α positions have equivalent positions in the two proteins despite the absence

5

of any sequence identity (Fig. 4b). The domain is about half the size of Bchl a which has a single domain structure without major extensions. Like Bchl a, the shape of the N-terminal domain resembles an envelope (or Taco) with a hollow inside and in Bchl a, 7 bacteriochlorophylls are buried in this cavity. However, the domain is not as hollow as BChl a since loop 135-155, which contains a small helical segment, is turned inwards and fills up the core. In BChl a the equivalent loop (290–305) is positioned more towards the exterior of the protein, thereby leaving space for some of the tertrapyrroles of the bacteriochlorophylls. The large sheet (17 strands) of Bchl a is truncated to only 7 strands in LTA4 hydrolase. Especially the region between residue 35 and 263 of Bchl a has been replaced by a much shorter region in LTA4 hydrolase (res. 45 to 98) that forms the 3 stranded small B-sheet and the edge strand of the larger 7 stranded \beta-sheet. The structure of the other half of the molecule is almost completely conserved, except the insertion of two extra strands instead of loops in LTA4 hydrolase. The structural homology between Bchl a, a protein involved in light harvesting, and LTA4 hydrolase was certainly unexpected. In LTA4 hydrolase, the function of the N-terminal domain is not yet known, but one may speculate that it participates in binding to hydrophobic molecules or surfaces with a possible regulatory function. In mammalian 15-lipoxygenase, a similar function was proposed for an N-terminal B-barrel domain with structural homology to a corresponding C-terminal domain in mammalian lipases (Gillmor, S.A., Villasenor, A., Fletterick, R., Sigal, E. & Browner, M.F. Nature Struc. Biol. 4. 1003-1009 (1997)).

The connection from the N-terminal to the catalytic domain is very short, a strand from the 4 stranded β-sheet connects into a strand of a 5-stranded antiparallel β-sheet of the catalytic domain. The two sheets are closely packed and the interface is mainly hydrophobic in character with 14 hydrophobic residues contributing from the N-terminal domain and 11 from the catalytic domain. Hydrogen bonds occur between Gln116 and Ser264, Ser124 and Gln226, the backbone of Ser124 and Glu223, the backbone of Ser151 and Lys309, Lys153 and the backbone of Leu305 and indirectly through a water molecule between Tyr130 and the back-

25

5

bone of Val260. Two salt-bridges between His139 and Asp375 and between Arg174 and Asp257 complete the interactions made in this interface.

4.3 The catalytic domain contains the zinc binding site and is structurally similar to thermolysin

The structure of the catalytic domain (res. 210-450) is surprisingly similar to the structure of thermolysin (Fig. 5a & b) (Holmes, M. & Matthews, B. J. Mol. Biol. 160, 623-639 (1982)). When the amino acid sequence in this domain was compared with that of thermolysin, the sequence identity was found to be very low (essentially confined to the zinc binding motifs). However, the structural homology stretches out over the whole domain. Thus, no less than 146 Ca positions overlap with an r.m.s. deviation of 1.946 Å. Like thermolysin, the catalytic domain consists of two lobes, one mainly a-helical and one mixed a/b lobe. The a-lobe consists of 6 major helices interconnected by long loops containing smaller helical segments, while the a/b lobe has a 5 stranded mixed β-sheet lined with 3 helices on one side. The zinc binding site is found in between the two lobes. Since this domain contains only 245 amino acids and thermolysin contains 314 residues, some truncations have taken place, especially in the a/b lobe in which the N-terminal extended b structure is truncated and only a mixed 5 stranded β-sheet remains. The changes in the a-lobe are smaller. Here the long meandering loop 181 to 221 has been replaced by a long a-helix and the b-hairpin from 245 to 258 has been deleted.

A loop in extended conformation on the surface of the protein from 451 to 463 connects the catalytic domain with the C-terminal domain. Interestingly, this segment contains a highly conserved proline rich motif P451-G-f-P-P-x-K-P-x-Y460 which bears some resemblance to an SH3 domain recognition sequence. However, the canonical arginine residue is not present on either side of the proline motif. Nevertheless, since this stretch of amino acids is exposed on the surface of the protein, it is still possible that it could serve as an anchoring site for protein-protein interactions.

The C-terminal domain (464-610) is composed of 9 a-helices that form an unusual coil of helices reminiscent of the ones found in lytic transglycosylase⁴⁰ and

recently in the armadillo repeat region of b-catenin (Huber, A.H., Nelson, W.J. & Weis, W.I. Cell 90, 871-882 (1997)) (Fig. 6). The helices pack into two layers of parallel helices (5 inner and 4 outer helices) and in an anti-parallel manner between the two layers. The arrangements found in the two other proteins are much larger and form super-helical structures. In the C-terminal domain of LTA4 hydrolase, the arrangement is more straight and has a very compact shape. One of the helices is deformed and one of the interconnecting loops is long and contains a small 310 helix. The domain makes contacts with both the a-lobe of the catalytic domain and one of the edges of the N-terminal domain. It is positioned in a way such that the helices lie perpendicular to the 7 stranded b-sheet of the N-terminal domain and to most of the helices in the catalytic domain. The helices are amphipatic in character, with the hydrophobic sides towards the middle of the domain and hydrophilic residues pointing towards the solvent and into the deep cleft in the middle of the whole molecule. This side of the cleft is highly polar; 10 Arg and Lys residues and 4 Asp and Glu residues are positioned on this side.

4.4 Zinc coordination

The immediate surroundings of the active site Zn²⁺ ion are very similar in thermolysin and LTA4 hydrolase. The Zn²⁺ is bound between the two lobes and is coordinated by His295, His299, one carboxylic oxygen of Glu318 and the carbonyl and hydroxyl oxygens of the inhibitor bestatin so that a square based pyramid is formed. The two histidines originate from a long a-helix and the glutamate from a neighboring a-helix, all in the a-lobe. Glu296 and Tyr383, two residues implicated in the reaction mechanism for the peptide cleaving activity, are located near the Zn ion. Glu296, the putative general base, is positioned next to the metal ligand His295 and bends over the bestatin molecule and Tyr383, which was described as a proton donor, also makes contact with the bestatin molecule (Figure 8a).

Interestingly, the second layer around the Zn ion shows differences between thermolysin and LTA4 hydrolase. In both enzymes the orientation of the zinc binding ligands is fixed by hydrogen bonds, however the hydrogen bond acceptors are positioned differently. In thermolysin, the Nd1 of His142 is hydrogen bonded to the

20

25

5

Od2 of Asp170, while in LTA4 hydrolase the Nd1 of His295 is hydrogen bonded to the Oe1 of Glu325. This residue comes from a structural equivalent to the helix carrying Asp170 in thermolysin, but is shifted half a turn outwards. The Nd1 of His146 in thermolysin is hydrogen bonded to the Od1 of Asn165. This residue is part of the zinc binding signature and is conserved between the two enzymes. However, in LTA4 hydrolase the helix in which this conserved residue is placed has been rotated slightly and Asn317 is no longer making a hydrogen bond to His299. The orientation of His299 is now fixed by a hydrogen bond from the Nd1 to the carbonyl backbone oxygen of Thr302. The Od1 of Asn317 makes instead a hydrogen bond to the backbone amide of Asn381 while the Nd2 makes a hydrogen bond to the hydroxyl group of Tyr200. The last protein-ligand, Glu166 is in thermolysin hydrogen bonded to Tyr157 and a water molecule, in LTA4 hydrolase, Glu318 is only hydrogen bonded to a water molecule (Fig. 7).

4.5 Bestatin binding

Although the zinc binding site is formed by residues only from the catalytic domain and most catalytic residues also come from this domain, the active site itself is surrounded by loops from all three domains. The binding of bestatin reflects this, since it makes interactions with residues from all three domains. The main interactions of bestatin are made through the carbonyl and hydroxyl oxygens to the Zn atom. Hydrophobic interactions are made between the phenyl moiety and the phenyl rings of Tyr267, Phe316, Tyr378 and Tyr383. Also, Met270 and Gln136 are involved (Fig. 8a). The other end of the inhibitor is pointing towards the solvent, the leucine moiety makes interactions with Val292 and His295, while the carboxylic oxygens make interactions with Arg563 and Lys565 through water molecules as well as hydrogen bonds to the backbone nitrogen atoms of Gly268 and Gly269. Hydrogen bonds are formed between the peptidyl N of bestatin and Oe2 of Glu296 and between the terminal NH2 and the Oe1 of Glu271 and Oe1 of Gln136. The hydroxyl oxygen makes apart from the interaction with the Zn ion also an interaction to the OH of Tyr383. (For schematic overview see Fig. 8b). Tyr378 which gets modified during suicide inactivation sits slightly further away, but makes a hydrogen bond to Tyr383 and some hydrophobic interactions with the phenyl ring of the

20

25

5

inhibitor. These two tyrosine are both found on the same stretch of amino-acids that in thermolysin form a long a helix, however in leukotriene hydrolase this helix is interrupted and two turns of the helix are replaced by three residues (378-380) in an extended conformation. The binding of bestatin is quite different as was found in the complex between bestatin and bovine lens leucine amino-peptidase (blLAP) (Burley, S., David, P., Sweet, R., Taylor, A. & Lipscomb, W. J. Mol. Biol. 224, 113-140 (1992)). In that complex, bestatin was bound to the Zn by both the terminal nitrogen and the nonproteinaceous P1 hydroxyl oxygen, while in LTA4 hydrolase the bestatin is bound by the hydroxyl and carbonyl oxygens. The terminal nitrogen is involved in hydrogen bonding to Glu271 and Gln136. These differences could stem from the fact the blLAP is a bimetal protein with a different reaction mechanism. Moreover the binding of bestatin as seen in LTA4 hydrolase is similar with the complexes formed between thermolysin and hydroxamates which also act as bidentate ligands by the hydroxyl and carbonyl oxygens (Holmes, M. & Matthews, B. Biochemistry 20 (1981)).

Behind the pocket in which the phenyl ring of bestatin binds, there is a cavity that stretches 15 Å deeper into the protein and is approximately 6 to 7 Å wide. In the present structure this cavity is filled with water molecules. It has however a very hydrophobic nature and is lined with Trp311, Phe314, Trp315 Phe362, Leu365, Val367, Leu369, Pro374, Ala377, Tyr378, and Pro382. Most of these residues are strictly conserved or conserved in nature in all LTA4 hydrolase sequences known up until now, with the exception of Val367, which is replaced by a Gln in the yeast and *C. elegans* sequences. Interestingly space for this cavity is partly created by the interruption by the extended conformation in the stretch where Tyr378 and Tyr383 are found. One patch of this binding site is quite hydrophilic with Asn134, Asp375 and the OH of Tyr267 clustering together. This bigger cavity could be a binding site for the LTA4 substrate molecule. If the epoxide moiety would bind in a similar way as the carbonyl oxygen of bestatin to the Zn ion, then the hydrophobic tail would fit snugly into the binding site now occupied by the phenyl group of bestatin and

25

5

would continue into the deeper hydrophobic cavity (Fig. 9a). The other tail would sit in the pocket that is now occupied by the carboxy group of bestatin and it would be long enough for the carboxylic acid to make direct electrostatic interactions with the conserved Arg563 and Lys565.

The replacement of Val367 by Gln as seen in the enzyme from yeast would make the hydrophobic channel shorter and this might be one of the reasons why the yeast enzyme has a poor leukotriene A4 epoxide hydrolase activity. The manner in which the leukotriene molecule would bind is similar as what is proposed for binding of arachidonic acid in 15-lipoxygenase (Gillmor, S.A., Villasenor, A., Fletterick, R., Sigal, E. & Browner, M.F. *Nature Struc. Biol.* 4, 1003-1009 (1997)) with the hydrophobic end buried inside the protein and the carboxylic acid more towards the surface making interactions with Arg and Lys residues.

The binding of bestatin acts also as a guide for the binding of peptide substrate molecules. From systematic binding studies with tri-peptides it was shown that the enzyme has a strong preference for an arginine residue as the N-terminal residue and for several tri-peptides the enzyme has a kcat/Km ratio 10-fold the kcat/Km for LTA4 (Örning, L., Gierse, J.K. & Fitzpatrick, F.A. J. Biol. Chem. 269, 11269-11273 (1994). If we roughly model a peptide in the active site with an N-terminal Arg with the carbonyl oxygen sitting on the place of the hydroxyl group of bestatin, then the Arg side-chain of this residue would sit in the same place as the phenyl group of the bestatin with the guanidinium headgroup interacting with the conserved Asp375 and the OH of Tyr267 and the more hydrophobic Cb, Cd and Cg atoms making similar interactions as the phenyl ring. The terminal aminogroup could make the same electrostatic interaction as the terminal aminogroup of bestatin with Asp271 and Gln136. This mode of binding of bestatin is in contrast with the mode proposed by Örning, since the phenyl ring seems to occupy the S1 pocket. We also propose that the LTA4 substrate molecule is occupying all three pockets, S1, S'1 and S'2.

If the binding mode of peptides in LTA4 hydrolase is compared with the one described for thermolysin, a number of differences are observed. In thermolysin, the

25

5

peptide molecule is held in place by many interactions to the main chain atoms provided by Asn112, Ala203, Arg203 and Trp115. None of these residues or equivalent residues can be found in the binding site in LTA4 hydrolase. Furthermore, although binding pockets S1 and S'1 are at similar positions as in thermolysin, site S'2 has to be different since its space is occupied by Tyr378 in LTA4 hydrolase. Glu271 and Gln136 and the N-terminal domain are filling up the space into which in thermolysin the upstream peptide binds contributing to the exo-peptidase function instead of an endo-peptidase function as in thermolysin.

4.6 Putative Phosphorylation site

Recently specific phosphorylation by a yet unknown specific kinase of Ser415 has been described as means of regulation of LTA4 hydrolase activity in endothelial cells (Rybina, I.V., Liu, H., Gor, Y. & Feinmark, S.J. *J Biol Chem* 272, 31865-71 (1997)). This residue is conserved in all mammalian LTA4 hydrolases and is embedded in a highly homologous stretch of residues. Phosphorylation of this residue seems to inhibit the epoxide hydrolase activity but not the amino-peptidase activity. In the structure this residue is located in a loop connecting two a-helices that lie on the surface of the molecule. The loop itself is located at the back of the enzyme.

4.7 Aminopeptidase activity

The amino-peptidase activity catalyzed by this enzyme has been well studied and many of the important residues have been target for site-directed mutagenesis work. This lead to a proposal in which Glu296 would act as a general base (Wetterholm, A., et al. Proc Natl Acad Sci U S A 89, 9141-9145 (1992)) and Tyr383 as a putative proton donor (Blomster, M., Wetterholm, A., Mueller, M.J. & Haeggström, J.Z. Eur. J. Biochem. 231, 528-534 (1995)). In the current complex, these residues are involved in hydrogen bonds with the bestatin molecule. If bestatin binding is seen as a rough analog for the transition state binding, then the interaction of Glu296 with the hydroxyl oxygen of bestatin indicates that this residue could indeed activate a water-molecule for the nucleophilic attack. The role of Tyr383 cannot so easily be confirmed, however its position strongly suggest the role of proton donor. In thermolysin the proton donor is His231 and although the Ca position of this resi-

5

due is 4.1Å removed from the Ca position of Tyr383 in LTA4 hydrolase, the Nd1 is only 1 Å removed from the OH position of Tyr383. The conserved Glu271 could be involved in the exo-protease activity of the protein. Recently, the analogous Glu350 in aminopeptidase N and Glu352 in aminopeptidase A were subject to site-directed mutagenesis work (Luciani, N., et al. Biochemistry 37, 686-692 (1998); and Vazeux, G., Iturrioz, X., Corvol, P. & Llorenz-Cortez, C. Biochem. J. 334, 407-413 (1998)) and it was observed that mutations of this residue lead to large decreases in the activity in the case of substitutions by conserved amino-acids such as aspartate and glutamine and absence of activity in substitution by alanine. It was concluded that Glu350 belonged to the anionic binding site in that protein. A mechanism based on thermolysin was proposed for aminopeptidase N with a pentavalent transition state with an additional interaction between the free a-aminogroup and Glu350. In this structure we can observe such an interaction between Glu271 and the free aminogroup of bestatin. Furthermore the penta-valent coordination of Zn by the His295, His299, Glu318 and the carbonyl and hydroxyl groups of bestatin indicates that this is an equivalent transition state analog complex as determined previously for thermolysin.

From careful sequence alignments and structural insight we can conclude that the enzymes in the M1 family of proteases will share a highly conserved catalytic domain that includes part of the N-terminal domain as we see it in LTA4 hydrolase and the thermolysin-like domain. There is no homology for residues in the C-terminal domain and we believe that this domain is unique for LTA4 hydrolases. According to the present invention, it is suggested that all proteases belonging to class M1 with the signature HExxH and a Glu 18 residues downstream will function in a similar way to thermolysin.

4.8 Epoxide hydrolase activity

Concerning the epoxide hydrolase activity, much less is known about the functional elements and mechanisms of catalysis. In fact, the prosthetic zinc is the only critical component identified thus far and may potentially assist in the introduction of a water molecule at C12 or in the activation of the epoxide. Although Tyr378 and

25

5

Tyr383 are important active side residues, none of them is essential for catalysis. A mutation of Tyr378 to Phe protects the enzyme against suicide inhibition, however the specificity of the double bond configuration is partly lost (Mueller, M., Andberg, M., Samuelsson, B. & Haeggstrom, J. J. Biol. Chem. 271, 24345-24348 (1996)) since a novel metabolite with a cis-trans-cis conjugated system can be detected. Thus, Tyr378 is a major binding site for LTA4 during suicide inactivation and seems to play a role for the formation of the correct double bond geometry in the product LTB4. Mutations of Tyr383 abolish the amino-peptidase activity where it has a role as potential proton donor (vide supra) but the epoxide hydrolase activity is only decreased compared to wild-type. It is however implicated in the stereospecific introduction of water during the hydrolysis of LTA4 to LTB4 since these mutants convert LTA4 in both LTB4 and 5 [S],6 [S]-DHETE (Andberg, M., Hamberg, M. & Haeggstrom, J. J. Biol. Chem. 272, 23057-23063 (1997)). Moreover careful analysis of the catalytic properties of enzymes mutated in pos. 383, viz [Y383F], [Y383H] and [Y383Q]LTA4 hydrolase have indicated that the epoxide hydrolase reaction follows an SN1 mechanism.

If one considers the chemistry carried out by LTA4 hydrolase, the enzyme has two major tasks during the hydrolysis of LTA4 to LTB4. First introduction of a water molecule stereospecific at C12 and second to generate a cis-double bond Æ6 in the resulting conjugated triene system [cf. Fig. 1]. If LTA4 is modeled into the putative substrate binding pocket as indicated in figure 9b, the catalytic zinc gets close to the epoxide and not C12 of the substrate. Therefore the most likely role of the Zn ion is to act directly as a Lewis acid to activate and open the epoxide ring. This would generate a carbocation, whose charge will be delocalised over the conjugated triene system from C7 to C12. Since this intermediate has an sp2 hydridized planar configuration at C12, it is in principle open for nucleophilic attack from either side of the molecule. The conserved Asp375 is positioned in such a way that a water molecule bound to it is in "attacking" distance of C12 of a modeled LTA4 molecule, the position into which a hydroxyl group is inserted during the reaction.

10

15

20

25

This will account for the proper stereo-chemical and positional insertion of the hydroxyl-group at C12 in R configuration.

The shape and curvature of the LTA4 binding pocket also gives a clue as to how the enzyme creates the cis double bond at Æ6. Since there is free rotation between the c6 and c7 of LTA4, this bond may be kept in a "pro-cis" configuration in the transition state, which in turn would facilitate the formation of a Æ6-cis double bond form the carbocation intermediate. If LTA4 is modeled in this way, the entire molecule adopts a bent shape, fitting very well with the architecture of the binding pocket (Fig. 9b). Hence, the critical double bond geometry at Æ6 of LTB4 is probably guaranteed by the exact binding conformation of LTA4 at the active side which in turn is governed by all the structural elements participating in substrate binding. including the carboxylate recognition sites, Arg56 and Lys565, the catalytic zinc and the hydrophobic residues lining the pocket. The putative binding cleft for the leukotriene molecule is narrow and bend and thereby favoring LTA4 over other epoxides. The two tyrosines are positioned such that they are in contact with the triple double bond configuration of a modeled LTA4 molecule at the bent of the putative binding pocket and they are hydrogen-bonded to each other. Therefore their position is ideal for guidance in stereo-specificity of the double bond configuration. The loss of specificity for the hydroxyl-incorporation at the C12 position in case of the Tyr383 position can be explained that mutations at this position would possibly create extra space for a water molecule that could attack at the C6 position and thereby form 5 [S],6 [S]-DHETE.

The position of Tyr378 is such that it is in contact with the C6 atom of the modeled LTA4 molecule. If after opening of the epoxide ring the hydroxyl group of Tyr378 instead of a water molecule would attack the carbon-cation at the C6 position, a covalently attached molecule is formed which forms the suicide inhibited complex. In order to check this hypothesis and to obtain more information about the binding-site for leukotriene A4, the structure of this inhibited species would be essential.

49 WO 00/50577 PCT/SE00/00384

In order to exclude the possibility that residues near the active site might have further catalytic roles in the epoxide hydrolase reaction, a thorough investigation of these residues, such as Glu271 and Gln136 has to be started. Furthermore the proposed role of Asp375 in activating a water molecule for the stereospecific attack at C12 has to be investigated.

Accordingly, the present invention has solved the first specific leukotriene converting enzyme, which for the first time reveals the binding mode for leukotriene molecules. Furthermore, insight is provided in a unique active site that harbours two activities using different amino-acids to catalyze different reactions.

5. CONFORMATIONAL DATA

Table 9: Structure coordinates of LTA₄ hydrolase-thiolamine complex

	[4]	activities using different amino-acids to catalyze different reactions.												
	J 10													
SCALE1	10													
SCALE1	To sail	<u>5. CONF</u>	<u>'ORN</u>	<u>MAT</u>	<u>ION</u>	Λ L	DATA							
SCALE1	1=k	T	able	9: Str	ructu	re	coordinate	s of LTA	hvdrola	se-thiola	mine c	omnley		
SCALE1	(se unora	unine c	ompiex		
SCALE3	upijane u ram		68.			.15				90.00	P21212	2		
Atom res. Chain No. x y z occ B-factor Atom res. Chain No. x y z occ B-factor Atom res. Chain No. x z z occ B-factor Atom res. Chain No. x z z occ B-factor Atom res. Chain No. 1 - 1.1.890	15													
Atom res. Chain No. x y z occ B-factor 20	## 13													
Atom res. Chain No. x y z occ B-factor 20 ATOM 1 N PRO A 1 -0.593 16.387 63.494 1.00 97.99 ATOM 2 CA PRO A 1 -1.890 16.918 63.874 1.00 97.22 ATOM 3 C PRO A 1 -2.210 18.371 63.525 1.00100.00 ATOM 4 O PRO A 1 -2.210 18.371 63.525 1.00100.00 ATOM 5 CB PRO A 1 -2.130 16.551 65.383 1.00100.00 ATOM 6 CG PRO A 1 -2.130 16.551 65.383 1.00100.00 ATOM 7 CD PRO A 1 -0.290 15.233 64.369 1.00 97.81 ATOM 8 N GIU A 2 -2.216 19.272 64.556 1.00 96.95 ATOM 9 CA GLU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 10 C GIU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 11 O GIU A 2 -2.512 21.542 66.562 1.00 93.21 ATOM 12 CB GLU A 2 -4.105 20.768 64.214 1.00 97.26 ATOM 13 CG GIU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 14 CD GIU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 15 OEI GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 16 OE2 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 20 O ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CGI ILE A 3 0.308 24.324 65.707 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CDI ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 91.36 ATOM 29 CB VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 30 CGI VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 30 CGI VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56		SCALE3		0.0	0000		0.00000	0.0120	1	0.00000)			
ATOM				74			•••							
ATOM	fi.			Atom	res	. (Chain No.	x	У	Z	occ	B-factor		
ATOM 2 CA PRO A 1 -1.890 16.918 63.874 1.00 97.99 ATOM 3 C PRO A 1 -2.210 18.371 63.525 1.00100.00 ATOM 4 O PRO A 1 -2.210 18.371 63.525 1.00100.00 ATOM 5 CB PRO A 1 -2.402 18.667 62.342 1.00100.00 ATOM 6 CG PRO A 1 -2.130 16.551 65.332 1.00 97.81 ATOM 7 CD PRO A 1 -0.290 15.233 64.369 1.00 97.05 ATOM 8 N GLU A 2 -2.216 19.272 64.556 1.00 96.95 ATOM 9 CA GLU A 2 -2.169 20.678 64.314 1.00 95.71 ATOM 10 C GLU A 2 -2.188 21.701 65.386 1.00 94.33 ATOM 11 O GLU A 2 -2.188 21.701 65.386 1.00 94.33 ATOM 12 CB GLU A 2 -4.567 21.732 63.125 1.00100.00 ATOM 13 CG GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 14 CD GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 15 OEI GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 16 OE2 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 75.668 ATOM 21 CB ILE A 3 -1.148 23.905 65.820 1.00 83.63 ATOM 22 CG1 ILE A 3 -0.842 65.707 1.00 83.45 ATOM 24 CD1 ILE A 3 -1.150 25.521 64.759 1.00 83.63 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 27 C VAL A 4 -1.725 26.099 66.523 1.00 50.98 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 31 CG2 VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 31 CG2 VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56		атом	1	N	חחת	70	3	0 500	1.5 5.5					
ATOM 3 C PRO A 1 -2.210 18.371 63.525 1.00100.00 ATOM 4 O PRO A 1 -2.402 18.667 62.342 1.00100.00 ATOM 5 CB PRO A 1 -2.402 18.667 62.342 1.00100.00 ATOM 6 CG PRO A 1 -2.130 16.551 65.332 1.00 97.81 ATOM 7 CD PRO A 1 -1.221 15.355 65.583 1.00100.00 ATOM 8 N GLU A 2 -2.216 19.272 64.556 1.00 96.95 ATOM 9 CA GLU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 10 C GLU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 11 O GLU A 2 -2.188 21.701 65.386 1.00 94.33 ATOM 12 CB GLU A 2 -2.188 21.701 65.386 1.00 94.33 ATOM 13 CG GLU A 2 -4.105 20.768 64.214 1.00 97.26 ATOM 14 CD GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 15 OEI GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 16 OE2 GLU A 2 -3.301 21.261 61.52 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 19 C ILE A 3 -2.066 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 40 ATOM 21 CB ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 22 CG1 ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.725 26.099 66.523 1.00 50.98 ATOM 29 CB VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.40 ATOM 30 CG1 VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	F 1													
ATOM	किंद्र सर्वे र स्था सर्वे ४										1.00	97.22		
25 ATOM	Sec.										1.001	100.00		
25 ATOM 6 CG PRO A 1 -1.221 15.355 65.583 1.00100.00 ATOM 7 CD PRO A 1 -0.290 15.233 64.369 1.00 97.05 ATOM 8 N GLU A 2 -2.216 19.272 64.556 1.00 96.95 ATOM 9 CA GLU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 10 C GLU A 2 -2.512 21.542 66.562 1.00 93.21 ATOM 11 O GLU A 2 -2.512 21.542 66.562 1.00 93.21 ATOM 12 CB GLU A 2 -4.105 20.768 64.214 1.00 97.26 ATOM 13 CG GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 14 CD GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 15 OE1 GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 16 OE2 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.99 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.99 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.99 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	iber dise									62.342				
ATOM 7 CD PRO A 1 -0.290 15.233 64.369 1.00 97.05 ATOM 8 N GLU A 2 -2.216 19.272 64.556 1.00 96.95 ATOM 9 CA GLU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 10 C GLU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 11 O GLU A 2 -2.188 21.701 65.386 1.00 94.33 ATOM 11 O GLU A 2 -2.512 21.542 66.562 1.00 93.21 ATOM 12 CB GLU A 2 -4.105 20.768 64.214 1.00 97.26 ATOM 13 CG GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 14 CD GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 15 OEI GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 16 OE2 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CGI ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CDI ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 29 CB VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 29 CB VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CGI VAL A 4 -3.735 28.754 68.047 1.00 58.99 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	25													
ATOM 8 N GLU A 2 -2.216 19.272 64.556 1.00 96.95 ATOM 9 CA GLU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 10 C GLU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 11 O GLU A 2 -2.512 21.542 66.562 1.00 93.21 ATOM 12 CB GLU A 2 -4.155 20.768 64.214 1.00 97.26 ATOM 13 CG GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 14 CD GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 15 OEI GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 16 OE2 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.036 25.154 65.661 1.00 75.68 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CGI ILE A 3 0.452 25.218 64.763 1.00 76.97 ATOM 23 CG2 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -2.477 27.303 66.482 1.00 50.98 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CGI VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CGI VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56														
ATOM 10 C GLU A 2 -2.569 20.678 64.314 1.00 95.71 ATOM 11 O GLU A 2 -2.512 21.542 66.562 1.00 93.21 ATOM 12 CB GLU A 2 -4.105 20.768 64.214 1.00 97.26 ATOM 13 CG GLU A 2 -4.105 20.768 64.214 1.00 97.26 ATOM 14 CD GLU A 2 -4.57 21.732 63.125 1.00100.00 ATOM 15 OEI GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 16 OE2 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.45 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 29 CB VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38											1.00	97.05		
ATOM 10 C GLU A 2 -2.188 21.701 65.386 1.00 94.33 ATOM 11 O GLU A 2 -2.512 21.542 66.562 1.00 93.21 ATOM 12 CB GLU A 2 -4.105 20.768 64.214 1.00 97.26 ATOM 13 CG GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 14 CD GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 15 OE1 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 16 OE2 GLU A 2 -5.361 20.398 61.368 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.308 24.324 65.707 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 27 C VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 28 O VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38							2							
ATOM 11 O GLU A 2 -2.512 21.542 66.562 1.00 93.21 ATOM 12 CB GLU A 2 -4.105 20.768 64.214 1.00 97.26 ATOM 13 CG GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 14 CD GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 15 OE1 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 16 OE2 GLU A 2 -5.361 20.398 61.368 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -2.477 27.303 66.482 1.00 50.98 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 31 CG2 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38														
ATOM 12 CB GLU A 2 -4.105 20.768 64.214 1.00 97.26 ATOM 13 CG GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 14 CD GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 15 OE1 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 16 OE2 GLU A 2 -5.361 20.398 61.368 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 98.40 ATOM 30 CG1 VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.99 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	30						2				1.00	94.33		
ATOM 13 CG GLU A 2 -4.587 21.732 63.125 1.00100.00 ATOM 14 CD GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 15 OEI GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 16 OE2 GLU A 2 -5.361 20.398 61.368 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38														
ATOM 14 CD GLU A 2 -4.351 21.139 61.767 1.00100.00 ATOM 15 OE1 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 16 OE2 GLU A 2 -5.361 20.398 61.368 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38														
35 ATOM 15 OE1 GLU A 2 -3.301 21.261 61.152 1.00100.00 ATOM 16 OE2 GLU A 2 -5.361 20.398 61.368 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -2.477 27.303 66.482 1.00 50.98 ATOM 28 O VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38							2							
ATOM 16 OE2 GLU A 2 -5.361 20.398 61.368 1.00100.00 ATOM 17 N ILE A 3 -1.550 22.799 64.944 1.00 86.29 ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -2.477 27.303 66.482 1.00 50.98 ATOM 28 O VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.56 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38							2							
ATOM 17 N ILE A 3	35			OE2	GLU	Α	2							
ATOM 18 CA ILE A 3 -1.148 23.905 65.820 1.00 81.53 ATOM 19 C ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38									22.799					
ATOM 20 O ILE A 3 -2.006 25.154 65.661 1.00 75.68 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38								-1.148	23.905					
40 ATOM 20 O ILE A 3 -2.835 25.288 64.763 1.00 76.97 ATOM 21 CB ILE A 3 0.308 24.324 65.707 1.00 83.45 ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.63 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38							3		25.154	65.661				
ATOM 22 CG1 ILE A 3 0.452 25.521 64.759 1.00 83.45 ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	40													
ATOM 23 CG2 ILE A 3 1.198 23.160 65.300 1.00 84.76 ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	40										1.00	83.45		
ATOM 24 CD1 ILE A 3 -0.184 25.361 63.375 1.00 91.36 ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38											1.00	83.63		
ATOM 25 N VAL A 4 -1.725 26.099 66.523 1.00 61.54 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38											1.00	84.76		
45 ATOM 26 CA VAL A 4 -2.477 27.303 66.482 1.00 56.32 ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38					ILE	A								
ATOM 27 C VAL A 4 -1.658 28.552 66.623 1.00 50.98 ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	45													
ATOM 28 O VAL A 4 -0.803 28.694 67.512 1.00 47.84 ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	70													
ATOM 29 CB VAL A 4 -3.514 27.318 67.595 1.00 58.99 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38														
50 ATOM 30 CG1 VAL A 4 -3.735 28.754 68.047 1.00 58.40 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	• ,													
50 ATOM 31 CG2 VAL A 4 -4.819 26.691 67.131 1.00 58.56 ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38														
ATOM 32 N ASP A 5 -2.012 29.486 65.732 1.00 39.38	50										1.00	58.40		
7006														
1.403 30.762 63.763 1.00 32.64									49.480 30 702		1.00	39.38		
						-•	•	1.100	30.702	05.763	1.00	32.04		

		MOTA	34	С	ASP A	. 5	6	-2.308	31.596	66.634	1.00	36.35
		MOTA	35	0	ASP A			-3.343	32.051	66.171	1.00	38.30
		MOTA	36	CB	ASP A			-1.252	31.492	64.400		30.79
		MOTA	37	CG	ASP A	. 5	5	-0.251	32.581	64.563	1.00	29.96
	5	MOTA	38		ASP A				33.123	65.635		35.01
		MOTA	39	OD2	ASP A				32.831	63.493		29.81
		ATOM	40	N	THR A				31.745	67.903		32.32
		MOTA	41	CA	THR A				32.507	68.842		32.08
		ATOM	42	С	THR A				34.011	68.557	1.00	40.63
	10	ATOM	43	0	THR A				34.759	69.132		46.68
		MOTA	44	CB	THR A				32.171	70.295		44.71
		ATOM	45		THR A				32.322	70.505		51.05
		ATOM	46		THR A				30.741	70.604		35.79
		ATOM	47	И	CYS A				34.480	67.656		32.51
	15	ATOM	48	CA	CYS A				35.923	67.335		28.92
		ATOM	49	C	CYS A			•	36.329	66.129		31.49
		ATOM	50	0	CYS A				37.523	65.875		25.42
gareg.		MOTA	51	CB	CYS A				36.410	67.107		27.38
ED		MOTA	52	SG	CYS A				35.944	68.518		32.02
AL.	20	MOTA	53	N	SER A				35.315	65.383		34.03
		ATOM	54	CA	SER A				35.508	64.158		32.97
1 a 1 a		ATOM	55	С	SER A				35.136	64.264		33.52
\$ 770 0 .		MOTA	56	0	SER A			-5.744	34.137	64.866		32.89
神神	0.5	ATOM	57	CB	SER A			-3.363	34.754	62.980		34.07
	25	ATOM	58	OG	SER A			-4.017	35.182	61.798		36.65
12 E		MOTA	59	N	LEU A			-6.289	35.921	63.635		30.79
H 40.		ATOM	60	CA	LEU A			-7.724	35.649	63.672		31.91
#		ATOM	61	С	LEU A		9	-8.198	35.009	62.377		36.07
12 10	20	MOTA	62	0	LEU A			-9.359	34.626	62.216		38.61
T.	30	ATOM	63	CB	LEU A		9	-8.514	36.958	63.874		32.47
		ATOM	64	CG	LEU A		9	-8.306	37.688	65.212		35.39
		MOTA	65		LEU A		9	-9.113	38.983	65.193		32.27
		ATOM	66.		LEU A			-8.746	36.816	66.397		33.25
	25	ATOM	67	N	ALA A			-7.273	34.933	61.443		28.63
J=40	35	MOTA	68	CA	ALA A			-7.545	34.408	60.147		27.14
		ATOM	69	C	ALA A			-7.643	32.921	60.090		34.34
		ATOM	70	0	ALA A			-7.296	32.173	61.005		37.34
		MOTA	71	CB	ALA A			-6.551	34.936	59.100		27.72
	40	ATOM	72	N	SER A			-8.130	32.503	58.959		32.08
	40	ATOM	73 74	CA	SER A			-8.256 6.838	31.115	58.708		32.03 32.67
		ATOM	75	C O	SER A	-		-6.838 -5.927	30.519 31.028	58.656 57.986		29.29
		ATOM ATOM	76	CB	SER A			-9.013	30.934	57.401		38.42
		ATOM	77	OG	SER A			-10.391	30.728	57.648		44.17
	45	ATOM	78		PRO A			-6.651	29.440	59.387		29.14
	-13	ATOM	79	CA	PRO A			-5.370	28.786	59.476		26.83
		ATOM	80	c.	PRO A			-4.935	28.176	58.173		32.64
		ATOM	81	Ö	PRO A			-5.737	28.007	57.284		35.89
		ATOM	82	ČВ	PRO A			-5.544	27.698	60.540		28.28
	50	ATOM	83	CG	PRO A			-7.029	27.571	60.843		32.92
		ATOM	84	CD	PRO A			-7.731	28.587	59.952		30.42
		ATOM	85	N	ALA A			-3.645	27.836	58.063		30.63
		ATOM	86	CA	ALA A			-3.066	27.236	56.855		28.36
		ATOM	87	Ç.	ALA A			-3.644	25.852	56.576		33.99
	55	ATOM	88	ŏ	ALA A			-3.455	25.240	55.528		31.60
		ATOM	89	СВ	ALA A			-1.561	27.133	57.050		27.68
		ATOM	90	N	SER A			-4.338	25.352	57.571		31.10
		ATOM	91	CA	SER A			-4.919	24.069	57.469		30.66
		MOTA	92	C	SER A			-6.242	24.133	56.753		37.86
	60	ATOM	93	ŏ	SER A			-6.768	23.118	56.328		45.79
		ATOM	94	СB	SER A			-5.005	23.386	58.825		34.33
		ATOM	95	OG	SER A			-6.006	23.978	59.621		41.01
		ATOM	96	N	VAL			-6.785	25.327	56.630		32.80
		ATOM	97	CA	VAL 2			-8.036	25.529	55.917		31.81

	MOTA	98	С	VAL A	15	-7,777	26.107	54.507	1.00 34.70
	ATOM	99	0	VAL A	15		25.576	53.494	1.00 31.96
	ATOM	100	CB	VAL A	15		26.336	56.720	1.00 33.07
	ATOM	101		VAL A	15		26.638	55.861	1.00 33.31
-5	ATOM	102		VAL A	15		25.538	57.949	1.00 30.32
,				CYS A	16		27.183	54.453	1.00 33.85
	ATOM	103	N						
	ATOM	104	CA	CYS A	16		27.826	53.189	1.00 38.27
	ATOM	105	С	CYS A	16		28.388	53.265	1.00 37.14
	ATOM	106	0	CYS A	16	-4.616	28.534	54.322	1.00 39.70
10	ATOM	107	CB	CYS A	16	-7.589	28.870	52.581	1.00 42.09
	ATOM	108	SG	CYS A	16	-7.844	30.418	53.540	1.00 47.38
	ATOM	109	N	ARG A	17	-4.679	28.722	52.132	1.00 32.10
	ATOM	110	CA	ARG A	17		29.262	52.101	1.00 32.54
	ATOM	111	C	ARG A	17		30.307	51.005	1.00 34.56
15	ATOM	112	ō	ARG A	17		30.065	49.842	1.00 35.07
13					17				
	MOTA	113	CB	ARG A			28.152	51.758	1.00 36.83
	ATOM	114	CG	ARG A	17		27.391	52.915	1.00 40.61
	ATOM	115	CD	ARG A	17		25.970	52.503	1.00 27.18
20	MOTA	116	NE	ARG A	17		25.026	53.501	1.00 52.41
20	ATOM	117	CZ	ARG A	17	* -1.244	24.036	54.035	1.00 69.41
42 20	ATOM	118	NH1	ARG A	17	0.020	23.812	53.683	1.00 54.86
ull.	ATOM	119	NH2	ARG A	17	-1.810	23.246	54.952	1.00 49.68
[-4 .	ATOM	120	N	THR A	18		31.454	51.378	1.00 27.06
, wa	ATOM	121	CA	THR A	18		32.477	50.428	1.00 26.12
25	ATOM	122	C	THR A	18		32.110	49.653	1.00 20.12
4 23									
	ATOM	123	0	THR A	18		31.964	50.194	1.00 29.06
ļaš.	MOTA	124	CB	THR A	18		33.810	51.134	1.00 34.27
	MOTA	125	OG1		18		34.261	51.738	1.00 32.95
	ATOM	126	CG2	THR A	18		34.839	50.156	1.00 35.91
30	MOTA	127	N	LYS A	19	-1.408	31.955	48.365	1.00 31.55
r.	MOTA	128	CA	LYS A	19	-0.298	31.615	47.511	1.00 31.74
Mi	ATOM	129	С	LYS A	19	0.359	32.848	46.906	1.00 33.90
	ATOM	130	0	LYS A	19		32.834	46.520	1.00 34.57
in the second	MOTA	- 131	CB	LYS A	19		30.697	46.398	1.00 36.08
35	ATOM	132	CG	LYS A	19		29.368	46.924	1.00 62.54
late .	ATOM	133	CD	LYS A	19		28.257	47.057	1.00 82.23
		134	CE	LYS A	19		27.880		
	MOTA							48.496	1.00 77.50
	ATOM	135	NZ	LYS A	19		27.849	48.745	1.00 55.63
40	ATOM	136	N	HIS A	20		33.928	46.810	1.00 31.40
40	MOTA	137	CA	HIS A	20		35.122	46.198	1.00 29.22
	ATOM	138	C	HIS A	20		36.345	46.517	1.00 34.68
	ATOM	139	0	HIS A	20		36.239	46.846	1.00 35.34
	MOTA	140	CB	HIS A	20	0.123	34.956	44.666	1.00 26.47
	ATOM	141	CG	HIS A	20	0.865	36.022	43.970	1.00 26.77
45	ATOM	142	ND1	HIS A	20	2.249	36.046	43.980	1.00 28.92
	MOTA	143	CD2	HIS A	20		37.091	43.280	1.00 27.43
	ATOM	144		HIS A	20		37.126	43.301	1.00 28.21
	ATOM	145		HIS A	20		37.781	42.865	1.00 28.18
	ATOM	146	N	LEU A	21		37.492	46.390	1.00 30.14
50		147	CA	LEU A	21		38.782		
50	ATOM							46.610	1.00 31.02
	ATOM	148	С	LEU A	21		39.786	45.562	1.00 38.34
	MOTA	149	0	LEU A	21		39.952	45.312	1.00 37.30
	MOTA	150	CB	LEU A	21		39.363	47.999	1.00 31.30
	MOTA	151	CG	LEU A	21		40.880	48.047	1.00 32.33
55	MOTA	152		LEU A	21		41.192	48.324	1.00 27.10
	ATOM	153	CD2	LEU A	21	0.277	41.522	49.100	1.00 32.86
	ATOM	154	N	HIS A	22		40.442	44.951	1.00 35.47
	ATOM	155	CA	HIS A	22		41.452	43.920	1.00 34.24
	ATOM	156	C	HIS A	22		42.742	44.550	1.00 33.99
60	ATOM	157	ō	HIS A	22		42.957	44.905	1.00 35.72
, 50	ATOM	158	CB	HIS A	22		41.244	42.624	1.00 33.72
	ATOM	159	CG	HIS A	22		42.256	41.615	1.00 35.97
	ATOM	160		HIS A	22		42.576	41.384	1.00 38.81
	MOTA	161	CD2	HIS A	. 22	-2.125	43.043	40.830	1.00 39.07

	ATOM	162	CE1	HIS A	22	-0.019	43.534	40.462	1.00 38.66
	ATOM	163		HIS A	22	-1.262	43.829	40.103	1.00 39.13
	ATOM	164	N	LEU A	23	-0.235	43.539	44.757	1.00 30.17
	ATOM	165	CA	LEU A	23	-0.416	44.793	45.405	1.00 33.32
5	ATOM	166	С	LEU A	23	-0.203	45.949	44.440	1.00 44.46
	ATOM	167	Ō	LEU A	23	0.828	46.068	43.761	1.00 44.06
	MOTA	168	СВ	LEU A	23	0.446	44.882	46.680	1.00 33.72
	ATOM	169	CG	LEU A	23	-0.141	45.682	47.871	1.00 33.15
	ATOM	170		LEU A	23	0.780	46.835	48.172	1.00 26.07
10	ATOM	171		LEU A	23	-1.539	46.213	47.609	1.00 35.39
	ATOM	172	N	ARG A	24	-1.256	46.765	44.395	1.00 42.83
	ATOM	173	CA	ARG A	24	-1.406	47.964	43.596	1.00 41.79
	ATOM	174	C	ARG A	24	-1.930	49.005	44.562	1.00 39.15
	ATOM	175	Ô	ARG A	24	-3.025	48.859	45.107	1.00 39.15
15	ATOM	176	CB	ARG A	24	-2.458	47.716	42.504	1.00 46.35
13	ATOM	177	CG	ARG A	24	-2.054	46.750	41.382	1.00 50.50
	ATOM	178	CD	ARG A	24	-2.754	47.058	40.043	1.00 80.27
	ATOM	179	NE	ARG A	24	-4.200	46.798	40.062	1.00 80.27
122		180	CZ	ARG A	24	-5.152	47.703	39.826	
175 20	ATOM	181		ARG A	24	-4.863	48.973	39.483	1.00100.00
20	ATOM								1.00100.00
42	ATOM	182		ARG A	24	-6.432	47.326	39.865	1.00100.00
}= 1 .	MOTA	183	N	CYS A	25	-1.164	50.028	44.844	1.00 32.39
TAN TAN	ATOM	184	CA	CYS A	25	-1.698	50.969	45.813	1.00 33.30
25	ATOM	185	С	CYS A	25	-1.061	52.325	45.724	1.00 34.82
25	ATOM	186	0	CYS A	25	-0.012	52.514	45.076	1.00 31.03
14 K	ATOM	187	CB	CYS A	25	-1.503	50.440	47.257	1.00 34.67
-A	MOTA	188	SG	CYS A	25	0.231	50.529	47.798	1.00 38.07
#	ATOM	189	N	SER A	26	-1.711	53.257	46.418	1.00 34.39
30	ATOM	190	CA	SER A	26	-1.196	54.601	46.437	1.00 36.77
30	ATOM	191	C	SER A	26	-0.963	55.133	47.821	1.00 39.85
n.	ATOM	192	0	SER A	26	-1.738	54.853	48.757	1.00 37.56
	ATOM	193	CB	SER A	26	-1.889	55.600	45.530	1.00 42.70
मुंब करि संब १८	ATOM	194	OG	SER A	26	-0.899	56.330	44.824	1.00 61.74
25	ATOM	195	N	VAL A	27	0.133	55.897	47.886	1.00 39.43
La 35	ATOM	196	CA	VAL A	27	0.624	56.583	49.081	1.00 41.31
	ATOM	197	C	VAL A	27	0.209	58.043	49.082	1.00 44.32
	ATOM	198	0	VAL A	27	0.562	58.799	48.187	1.00 45.24
	ATOM	199	CB	VAL A	27	2.135	56.531	49.207	1.00 46.35
40	ATOM	200		VAL A	27	2.524	57.207	50.522	1.00 45.62
40	ATOM	201		VAL A	27	2.592	55.079	49.178	1.00 47.20
	ATOM	202	N	ASP A	28	-0.553	58.417	50.093	1.00 37.94
	MOTA	203	CA	ASP A	28	-1.040	59.764	50.237	1.00 35.28
	ATOM	204	С 0	ASP A	28	-0.595	60.366	51.538	1.00 33.85
45	ATOM	205		ASP A	28	-1.181 -2.559	60.099	52.598	1.00 28.52
43	ATOM	206	CB	ASP A	28		59.807	50.189	1.00 37.09
	ATOM ATOM	207 208	CG OD1	ASP A	28 28	-3.055 -2.611	61.205 62.119	50.095 50.767	1.00 55.20 1.00 59.17
	ATOM	209		ASP A	28	-3.993			
	ATOM	210	N N	PHE A	29	0.436	61.335	49.192 51.405	1.00 61.41 1.00 36.42
50	ATOM	211	CA	PHE A	29		61.174 61.888	52.512	1.00 38.42
50	ATOM	212	C	PHE A	29		62.928	53.077	
	ATOM	213	Ö	PHE A	29		63.279	54.257	1.00 51.14 1.00 51.35
	ATOM	214	CB	PHE A	29		62.517	52.143	1.00 31.33
	ATOM	215	CG	PHE A	29		61.485	52.143	1.00 47.77
55	ATOM	216		PHE A	29				
25		217					60.957	53.247	1.00 52.08
	ATOM			PHE A	29		61.001	50.863	1.00 53.94
		218		PHE A	29		59.995	53.215	1.00 52.83
	ATOM ATOM	219 220	CE2	PHE A	29 29		60.046	50.813	1.00 56.46
60							59.538	51.992	1.00 53.39
00	ATOM	221	n ca	THR A	30		63.420	52.220	1.00 47.10
	ATOM ATOM	222 223	CA	THR A	30 30		64.386	52.654	1.00 45.48
		224					63.715	53.509	1.00 48.41
	MOTA	225	O CB	THR A	30 30		64.082	54.649	1.00 48.64
•	ATOM	223	CD	THR A	30	-2.283	65.097	51.434	1.00 54.06

	ATOM	226	OG1	THR A	30	-1.428	66.186	51.107	1.00 50.68
	ATOM	227	CG2		30	-3.697	65.568	51.745	1.00 60.28
		228							
	ATOM		N	ARG A	31	-3.392	62.683	52.978	1.00 46.66
_	ATOM	229	CA	ARG A	31	-4.404	61.987	53.734	1.00 47.88
5	ATOM	230	С	ARG A	31	-3.826	60.999	54.750	1.00 45.46
	ATOM	231	0	ARG A	31	-4.590	60.468	55.551	1.00 41.52
	ATOM	232	CB	ARG A	31	-5.335	61.214	52.805	1.00 56.73
		233	CG	ARG A					
	MOTA				31	-5.950	62.065	51.700	1.00 84.16
10	ATOM	234	CD	ARG A	31	-7.338	61.568	51.284	1.00100.00
10	MOTA	235	NE	ARG A	31	-7.344	60.450	50.327	1.00100.00
	MOTA	236	CZ	ARG A	31	-8.148	60.371	49.251	1.00100.00
	MOTA	237	NH1	ARG A	31	-9.034	61.324	48.944	1.00100.00
	ATOM	238		ARG A	31	-8.062	59.298	48.460	1.00100.00
1.5	ATOM	239	N	ARG A	32	-2.489	60.752	54.683	1.00 39.71
15	ATOM	240	CA	ARG A	32	-1.751	59.798	55.531	1.00 39.09
	ATOM	241	С	ARG A	32	-2.324	58.411	55.379	1.00 39.62
	MOTA	242	0	ARG A	32	-2.495	57.655	56.337	1.00 33.10
	ATOM	243	СВ	ARG A	32	-1.523	60.115	57.022	1.00 37.14
ಕ ವೆಯ			CG						
20	ATOM	244		ARG A	32	-1.197	61.569	57.337	1.00 71.25
20	ATOM	245	CD	ARG A	32	0.277	61.834	57.686	1.00100.00
in.	ATOM	246	NE	ARG A	32	0.703	61.299	58.986	1.00100.00
	ATOM	247	CZ	ARG A	32	1.284	62.005	59.961	1.00 79.51
44 ,	ATOM	248	NH1	ARG A	32	1.522	63.308	59.831	1.00 55.73
2 HG 17 E HG	ATOM	249		ARG A	32				
1 THE OF						1.626	61.387	61.098	1.00 44.96
25	MOTA	250	N	THR A	33	-2.612	58.068	54.139	1.00 39.83
	ATOM	251	CA	THR A	33	-3.162	56 .7 52	53.902	1.00 39.31
J=4.	MOTA	252	C	THR A	33	-2.543	56.010	52.760	1.00 41.13
9.77	MOTA	253	0	THR A	33	-1.853	56.574	51.926	1.00 42.93
#	MOTA	254	СВ	THR A	33	-4.635	56.835	53.641	1.00 43.44
30									
30	MOTA	255		THR A	33	-4.798	57.636	52.468	1.00 40.17
L me	MOTA	256	CG2	THR A	33	-5.245	57.468	54.880	1.00 38.71
	MOTA	257	N	LEU A	34	-2.822	54.717	52.762	1.00 35.26
14.1	ATOM	258	CA	LEU A	34	-2.372	53.799	51.745	1.00 35.20
100 mg	ATOM	259	С	LEU A	34	-3.632	53.293	51.098	1.00 32.49
35	ATOM	260	ō	LEU A	34				
						-4.474	52.670	51.751	1.00 30.96
	ATOM	261	CB	LEU A	34	-1.522	52.651	52.322	1.00 37.07
	ATOM	262	CG	LEU A	34	-0.149	52.571	51.685	1.00 42.99
	MOTA	263	CD1	LEU A	34	0.648	51.425	52.285	1.00 40.58
	ATOM	264	CD2	LEU A	34	-0.360	52.302	50.208	1.00 50.83
40	ATOM	265	N	THR A	35	-3.800	53.632	49.838	1.00 28.72
	ATOM	266	CA	THR A	35	-5.017	53.228	49.198	
									1.00 31.26
	ATOM	267	С	THR A	35	-4.838	52.329	48.013	1.00 36.54
	MOTA	268	0	THR A	35	-3.940	52.546	47.187	1.00 34.70
	ATOM	269	CB	THR A	35	-5.877	54.427	48.813	1.00 44.88
45	MOTA	270	OG1	THR A	35	-5.484	55.549	49.579	1.00 58.59
	MOTA	271		THR A	35	-7.324	54.094	49.109	1.00 49.42
	MOTA	272	N	GLY A	36	-5.726	51.329	47.950	
									1.00 32.57
	ATOM	273	CA	GLY A	36	-5.696	50.405	46.837	1.00 33.89
50	MOTA	274	С	GLY A	36	-6.418	49.074	46.993	1.00 34.50
50	ATOM	275	0	GLY A	36	-7.441	48.919	47.678	1.00 31.78
	MOTA	276	N	THR A	37	-5.836	48.103	46.293	1.00 35.93
	ATOM	277	CA	THR A	37	-6.327	46.723	46.281	1.00 36.12
	ATOM	278	C	THR A	37				
						-5.268	45.696	46.473	1.00 35.67
E E -	ATOM	279	0	THR A	37	-4.155	45.795	45.964	1.00 33.86
55	MOTA	280	CB	THR A	37	-7.119	46.306	45.050	1.00 42.21
	ATOM	281	OG1	THR A	37	-6.507	46.804	43.870	1.00 30.98
	ATOM	282	CG2	THR A	37	-8.547	46.793	45.229	1.00 50.03
	ATOM	283	N	ALA A	38	-5.687			
							44.705	47.220	1.00 32.95
60	ATOM	284	CA	ALA A	38	-4.886	43.570	47.533	1.00 33.45
60	MOTA	285	C	ALA A	38	-5.481	42.374	46.824	1.00 35.47
	ATOM	286	0	ALA A	38	-6.580	41.906	47.151	1.00 32.91
	ATOM	287	CB	ALA A	38	-4.845	43.341	49.044	1.00 33.72
	ATOM	288	N	ALA A	39	-4.764	41.874	45.834	1.00 32.70
	MOTA	289	CA	ALA A	39	-5.274	40.702	45.140	
	111011	ر ب ــ	₩	and A	39	5.2/1	30.702	42.T40	1.00 31.59

	MOTA	290	С	ALA A	39	-4.692	39.464	45.770	1.00	32.11
	ATOM	291	0	ALA A	39	-3.514	39.147	45.608	1.00	32.46
	ATOM	292	CB	ALA A	39	-4.934	40.729	43.662	1.00	32.13
	ATOM	293	N	LEU A	40	-5.505	38.774	46.508	1.00	27.06
- 5	ATOM	294	CA	LEU A	40	-5.001	37.593	47.155	1.00	29.04
	ATOM	295	C	LEU A	40	-5.331	36.322	46.364	1.00	36.88
	ATOM	296	0	LEU A	40	-6.485	36.100	45.963	1.00	28.89
	ATOM	297	CB	LEU A	40	-5.587	37.451	48.600	1.00	29.39
	ATOM	298	CG	LEU A	40	-5.303	38.598	49.559	1.00	31.39
10	ATOM	299	CD1	LEU A	40	-5.435	38.063	50.970	1.00	32.62
	ATOM	300	CD2	LEU A	40	-3.879	39.019	49.355	1.00	31.60
	ATOM	301	N	THR A	41	-4.310	35.470	46.165	1.00	42.40
	MOTA	302	CA	THR A	41	-4.523	34.210	45.488	1.00	43.93
	MOTA	303	C	THR A	41	-4.548	33.155	46.552	1.00	43.75
15	MOTA	304	0	THR A	41	-3.510	32.827	47.115	1.00	45.22
	ATOM	305	CB	THR A	41	-3.511	33.892	44.402	1.00	55.44
	MOTA	306	OG1	THR A	41	-3.604	34.885	43.418	1.00	55.57
	ATOM	307	CG2	THR A	41	-3.872	32.544	43.802	1.00	47.78
177	ATOM	308	N	VAL A	42	-5.755	32.688	46.848	1.00	33.25
20	ATOM	309	CA	VAL A	42	-5.946	31.720	47.893	1.00	32.21
% an . 	MOTA	310	С	VAL A	42	-6.166	30.312	47.380		40.56
	MOTA	311	0	VAL A	42	-6.827	30.105	46.376	1.00	42.56
1-1	MOTA	312	CB	VAL A	42	-7.017	32.153	48.920	1.00	36.45
ing me	MOTA	313	CG1	VAL A	42	-6.817	31.451	50.266	1.00	36.89
25	ATOM	314	CG2	VAL A	42	-6.963	33.665	49.170	1.00	36.10
UN.	MOTA	315	N	GLN A	43	-5.590	29.357	48.117	1.00	35.91
1.4.	ATOM	316	CA	GLN A	43	-5.678	27.945	47.838	1.00	31.59
*	ATOM	317	С	GLN A	43		27.244	48.988	1.00	38.98
	MOTA	318	0	GLN A	43	-5.916	27.317	50.144	1.00	40.92
30	ATOM	319	CB	GLN A	43	-4.305	27.319	47.568	1.00	30.50
Zp.	ATOM	320	CG	GLN A	43		25.800	47.259	1.00	53.80
	ATOM	321	CD	GLN A	43		25.177	47.099	1.00	62.47
12 m	ATOM	322	OE1		43		24.842	45.978		57.34
14 mg	ATOM	323	NE2		43		25.037	48.224		43.72
35	MOTA	324	N	SER A	44		26.555	48.664		33.83
4	MOTA	325	CA	SER A	44		25.839	49.678		31.38
	ATOM	326	С	SER A	44		24.557	50.117		42.10
	ATOM	327	0	SER A	44		23.814	49.292		42.78
40	ATOM	328	CB	SER A	44		25.530	49.226		28.60
40	ATOM	329	OG	SER A	44		24.785	50.224		34.57
	ATOM	330	N	GLN A	45		24.286	51.423		38.84
	MOTA	331	CA	GLN A	45		23.082	51.994		37.05
	ATOM	332	С	GLN A	45		22.050	52.269		47.57
45	ATOM	333	0	GLN A	45		20.917	52.678		42.94
45	ATOM	334	CB	GLN A	45		23.411	53.280		36.10
	ATOM	335	CG	GLN A	45		24.539	53.034		54.73
	MOTA	336	CD	GLN A	45		24.206	51.888		45.43
	ATOM	337		GLN A	45		24.888	50.833		39.23
50	MOTA	338	NE2		45		23.121	52.092		29.80
50	MOTA	339	N	GLU A	46		22.459	52.048		50.54
	ATOM	340	CA	GLU A	46		21.573	52.283		50.99
	ATOM	341	C	GLU A	46		21.583	51.179		54.49
	ATOM	342	0	GLU A	46		22.406	50.261		54.00
55	ATOM	343	CB	GLU A	46		21.793	53.657		51.61
ور	ATOM	344	CG	GLU A	46		22.979	54.454		55.93
	ATOM	345	CD	GLU A	46		23.329	55.646		78.67
	ATOM	346		GLU A	46		23.765	55.543		69.56
	ATOM	347		GLU A	46		23.129	56.796		75.10
60	ATOM	348	N	ASP A	47		20.630	51.300		48.90
00	ATOM	349	CA	ASP A	47		20.549	50.362		49.03
	ATOM	350	C	ASP A	47		21.425	50.846		55.15
	MOTA	351	0	ASP A	47		21.631	52.044		56.66
	MOTA	352	CB CG	ASP A	47		19.099	50.227		50.20
	MOTA	353	CG	ASP A	47	-13.083	18.376	49.218	T.00	66.88

	MOTA	354	OD1	ASP A	47	-12.340 1	18.945	48.434	1.00 66.27
	ATOM	355		ASP A	47		17.081	49.284	1.00 76.37
	ATOM	356	N	ASN A	48	-15.391 2	21.941	49.929	1.00 50.25
	ATOM	357	CA	ASN A	48	-16.519 2	22.755	50.339	1.00 48.45
5	ATOM	358	С	ASN A	48	-16.115 2	24.000	51.115	1.00 43.07
	ATOM	359	0	ASN A	48	-16.699 2	24.351	52.138	1.00 39.78
	ATOM	360	CB	ASN A	48	-17.559 2	21.909	51.117	1.00 51.19
	MOTA	361	CG	ASN A	48	-18.985 2	22.417	51.005	1.00 76.39
	ATOM	362	OD1	ASN A	48	-19.594 2	22.348	49.929	1.00 85.15
10	ATOM	363	ND2	ASN A	48	-19.515 2	22.928	52.115	1.00 68.29
	MOTA	364	N	LEU A	49		24.688	50.628	1.00 35.36
	MOTA	365	CA	LEU A	49	-14.728 2	25.874	51.335	1.00 34.40
	MOTA	366	С	LEU A	49	-15.601 2	27.009	50.851	1.00 47.38
	MOTA	367	0	LEU A	49	-15.421 2	27.515	49.734	1.00 45.47
15	MOTA	368	CB	LEU A	49	-13.239	26.152	51.173	1.00 31.04
	MOTA	369	CG	LEU A	49	-12.781	27.394	51.885	1.00 29.82
	MOTA	370	CD1	LEU A	49	-12.725	27.137	53.385	1.00 28.15
	ATOM	371	CD2	LEU A	49	-11.394	27.753	51.368	1.00 30.24
sil es.	MOTA	372	N	ARG A	50	-16.568	27.363	51.699	1.00 50.49
20	ATOM	373	CA	ARG A	50	-17.560	28.392	51.401	1.00 52.83
12	ATOM	374	С	ARG A	50	-17.169	29.838	51.702	1.00 55.57
il.	ATOM	375	0	ARG A	50	-17.627	30.760	51.011	1.00 53.89
j. 4.	ATOM	376	CB	ARG A	50	-18.928	28.028	51.986	1.00 58.35
25	ATOM	377	CG	ARG A	50	-19.863	27.354	50.980	1.00 74.76
25	ATOM	378	CD	ARG A	50	-20.438	26.024	51.462	1.00 81.60
Sid sist	ATOM	379	NE	ARG A	50	-21.214	25.355	50.415	1.00 94.37
u a	ATOM	380	CZ	ARG A	50	-22.465	24.888	50.538	1.00100.00
i i	ATOM	381	NH1	ARG A	50	-23.151	24.990	51.687	1.00100.00
₩.	ATOM	382	NH2	ARG A	50	-23.046	24.297	49.471	1.00 74.34
30	MOTA	383	N	SER A	51	-16.331	30.006	52.743	1.00 54.71
T.	ATOM	384	CA	SER A	51	-15.823	31.297	53.224	1.00 53.49
n.	ATOM	385	С	SER A	51	-14.495	31.156	53.955	1.00 53.57
1 m	MOTA	386	0	SER A	51	-14.146	30.062	54.420	1.00 52.93
\$4.00 \$6.00 \$4.00 \$6.00 \$4.00 \$6.00 \$4.00 \$6.00 \$4.00 \$4.00 \$4.00 \$4.00 \$4.00 \$4.00 \$4.00 \$4.00 \$4.00 \$4.00	MOTA	387	CB	SER A	51	-16.788	31.900	54.232	1.00 54.03
-35	MOTA	388	OG	SER A	51	-16.871	31.048	55.373	1.00 45.15
- A.	ATOM	389	N	LEU A	52		32.298	54.067	1.00 47.19
	ATOM	390	CA	LEU A	52	-12.519	32.422	54.762	1.00 45.66
	ATOM	391	С	LEU A	52	-12.415	33.671	55.640	1.00 50.43
	ATOM	392	0	LEU A	52		34.633	55.471	1.00 52.64
40	ATOM	393	CB	LEU A	52		32.117	53.923	1.00 44.20
	ATOM	394	CG	LEU A	52		33.044	52.745	1.00 43.98
	ATOM	395	CD1	LEU A	52		32.687	51.554	1.00 42.82
	ATOM	396	CD2	LEU A	52		34.501	53.094	1.00 44.71
	ATOM	397	N	VAL A	53	-11.483	33.658	56.579	1.00 44.97
45	ATOM	398	CA	VAL A	53	-11.271	34.781	57.455	1.00 41.69
	ATOM	399	С	VAL A	53		35.309	57.339	1.00 44.25
	MOTA	400	0	VAL A	53		34.551	57.302	1.00 45.42
	MOTA	401	CB	VAL A	53		34.420	58.906	1.00 45.48
50	ATOM	402		VAL A	53		35.554	59.853	1.00 44.94
50	MOTA	403		VAL A	53		34.073	59.050	1.00 45.79
•	MOTA	404	N	LEU A	54		36.627	57.166	1.00 35.12
	MOTA	405	CA	LEU A	54		37.333	57.080	1.00 34.14
	ATOM	406	С	LEU A	54		38.207	58.326	1.00 38.92
ا م م	ATOM	407	0	LEU A	54		38.457	59.108	1.00 37.45
55	ATOM	408	CB	LEU A	54		38.216	55.831	1.00 34.73
	ATOM	409	CG	LEU A	54		37.469	54.510	1.00 40.25
	ATOM	410		LEU A	54		38.488	53.374	1.00 40.69
	ATOM	411		LEU A	54		36.428	54.415	1.00 39.64
·	ATOM	412	N	ASP A	55		38.674	58.524	1.00 35.02
60	ATOM	413	CA	ASP A	55		39.526	59.627	1.00 31.65
	ATOM	414	С	ASP A	55		40.941	59.078	1.00 40.38
	ATOM	415	0	ASP A	55		41.151	57.886	1.00 39.98
	ATOM	416	CB	ASP A	55		39.232	60.075	1.00 30.92
	ATOM	417	CG	ASP A	55	-5.397	38.103	61.037	1.00 35.96

	ATOM	418	OD1	ASP A	55	-6.049	38.074	62.066	1.00 38.49
	ATOM	419		ASP A	55	-4.491	37.205	60.682	1.00 36.53
	ATOM	420	N	THR A	56	-7.196	41.900	59.963	1.00 42.93
	ATOM	421		THR A	56	-7.243	43.334	59.661	1.00 41.75
- 5	ATOM	422	C	THR A	56	-7.101	44.128	60.967	1.00 37.46
	ATOM	423	Õ	THR A	56	-7.517	43.687	62.049	1.00 37.40
	ATOM	424	СВ	THR A	56				
14						-8.514	43.825	58.894	1.00 37.17
	ATOM	425		THR A	56	-9.587	43.957	59.805	1.00 31.84
10	ATOM	426		THR A	56	-8.910	42.943	57.714	1.00 33.58
10	ATOM	427	N	LYS A	57	-6.513	45.304	60.863	1.00 26.63
	MOTA	428	CA	LYS A	57	-6.363	46.134	62.020	1.00 25.64
	MOTA	429	С	LYS A	57	-6.585	47.539	61.547	1.00 30.08
	MOTA	430	0	LYS A	57	-5.854	48.012	60.711	1.00 25.68
	MOTA	431	CB	LYS A	57	-4.991	45.983	62.641	1.00 27.34
15	MOTA	432	CG	LYS A	57	-4.907	46.387	64.100	1.00 35.83
	ATOM	433	CD	LYS A	57	-3.514	46.904	64.471	1.00 35.57
	ATOM	434	CE	LYS A	57	-2.901	46.225	65.689	1.00 50.54
	MOTA	435	NZ	LYS A	57	-2.521	47.180	66.757	1.00 55.43
eT m	ATOM	436	N	ASP A	58	-7.617	48.188	62.065	1.00 32.68
20	ATOM	437	CA	ASP A	58	-7.895	49.545	61.665	1.00 35.27
il -	ATOM	438	C	ASP A	58	-7.894	49.710	60.149	1.00 38.24
	ATOM	439	ō	ASP A	58	-7.289	50.627	59.571	1.00 35.86
į.	ATOM	440	CB	ASP A	58	-6.968	50.550	62.386	1.00 33.80
5 M/A	ATOM	441	CG	ASP A	58	-7.041	50.393	63.880	1.00 57.22
25									
4	ATOM	442		ASP A	58	-8.073	50.136	64.478	1.00 57.20
LT	ATOM	443		ASP A	58	-5.878	50.562	64.463	1.00 45.82
- 4w	ATOM	444	N	LEU A	59	-8.604	48.796	59.516	1.00 37.68
	MOTA	445	CA	LEU A	59	-8.720	48.813	58.079	1.00 39.36
3.20	ATOM	446	C	LEU A	59	-10.077	49.243	57.555	1.00 45.51
4 30	MOTA	447	0	LEU A	59	-11.146	48.946	58.120	1.00 44.18
T.	MOTA	448	CB	LEU A	59	-8.265	47.506	57.422	1.00 38.42
	MOTA	449	CG	LEU A	59	-6.762	47.475	57.218	1.00 37.40
7-7	MOTA	450		LEU A	59	-6.392	46.173	56.526	1.00 36.39
	MOTA	451	CD2	LEU A	59	-6.321	48.655	56.361	1.00 36.57
35	MOTA	452	N	THR A	60	-9.984	49.949	56.437	1.00 42.59
Į+A.	ATOM	453	CA	THR A	60	-11.132	50.483	55.734	1.00 42.63
	ATOM	454	С	THR A	60	-11.357	49.705	54.463	1.00 38.18
	MOTA	455	0	THR A	60	-10.632	49.856	53.454	1.00 34.33
	ATOM	456	CB	THR A	60	-11.030	52.028	55.532	1.00 65.15
40	ATOM	457	OG1	THR A	60	-11.806	52.736	56.504	1.00 67.56
	ATOM	458	CG2	THR A	60	-11.345	52.480	54.104	1.00 56.89
	ATOM	459	N	ILE A	61	-12.360	48.847	54.571	1.00 33.39
	ATOM	460	CA	ILE A	61	-12.753	47.975	53.482	1.00 35.89
	ATOM	461	C	ILE A	61	-13.726	48.634	52.533	1.00 41.05
45	ATOM	462	ō	ILE A		-14.913		52.840	1.00 40.08
	ATOM	463	CB	ILE A	61	-13.403	46.670	53.944	1.00 39.71
	ATOM	464		ILE A	61	-12.482	45.826	54.832	1.00 39.71
	ATOM	465		ILE A	61				
	ATOM	466		ILE A	61	-13.788 -11.027	45.900 45.851	52.691	1.00 38.96
50	ATOM							54.358	1.00 49.61
50		467	N	GLU A	62	-13.219	49.080	51.391	1.00 40.23
	MOTA	468	CA	GLU A	62	-14.040	49.700	50.365	1.00 41.73
	ATOM	469	C	GLU A	62	-14.986	48.633	49.826	1.00 47.09
	MOTA	470	0	GLU A	62	-16.207	48.726	49.926	1.00 47.52
55	ATOM	471	CB	GLU A	62	-13.138	50.272	49.239	1.00 44.08
55	ATOM	472	CG	GLU A	62	-13.765	51.406	48.381	1.00 64.08
	MOTA	473	CD	GLU A	62	-14.686	50.946	47.256	1.00100.00
	ATOM	474		GLU A	62	-15.458	50.002	47.376	1.00100.00
	ATOM	475	OE2	GLU A	62	-14.591	51.670	46.146	1.00 75.11
	ATOM	476	N	LYS A	63	-14.399	47.580	49.267	1.00 43.46
60	ATOM	477	CA	LYS A	63	-15.168	46.474	48.746	1.00 40.53
	ATOM	478	C	LYS A	63	-14.250	45.307	48.489	1.00 45.38
	ATOM	479	0	LYS A	63	-13.046	45.500	48.362	1.00 43.51
	ATOM	480	CB	LYS A	63	-15.818	46.830	47.428	1.00 40.46
	ATOM	481	CG	LYS A	63	-14.789	46.959	46.321	1.00 20.53

	ATOM	482	CD	LYS A	63	-15.367	47.555	45.054	1.00 28.36
	ATOM	483	CE	LYS A	63	-14.315	48.158	44.139	1.00 40.61
	MOTA	484	NZ	LYS A	63	-14.588	47.938		
								42.711	1.00 54.71
•	ATOM	485	N	VAL A	64	-14.862	44.116	48.441	1.00 45.57
5	MOTA	486	CA	VAL A	64	-14.190	42.844	48.171	1.00 44.90
	MOTA	487	С	VAL A	64	-14.666	42.263	46.841	1.00 46.44
	ATOM	488	0	VAL A	64	-15.826	41.917	46.700	1.00 45.81
	ATOM	489	СВ	VAL A	64	-14.505	41.748	49.192	1.00 46.24
		490		VAL A	64	-13.864			
10	ATOM						40.471	48.669	1.00 44.81
10	MOTA	491		VAL A	64	-14.040	42.048	50.627	1.00 44.77
	MOTA	492	N	VAL A	65	-13.793	42.099	45.875	1.00 43.10
	ATOM	493	CA	VAL A	65	-14.240	41.537	44.604	1.00 41.42
	ATOM	494	С	VAL A	65	-13.707	40.156	44.282	1.00 42.13
	ATOM	495	0	VAL A	65	-12.605	39.787	44.660	1.00 42.64
15	ATOM	496	СВ	VAL A	65	-13.856	42.462		
1.0								43.484	1.00 44.58
	ATOM	497		VAL A	65	-14.520	42.037	42.189	1.00 42.79
	ATOM	498	CG2	VAL A	65	-14.264	43.874	43.883	1.00 45.05
	ATOM	499	N	ILE A	66	-14.515	39.402	43.556	1.00 38.68
	MOTA	500	CA	ILE A	66	-14.179	38.053	43.113	1.00 39.98
20	ATOM	501	C	ILE A	66	-14.899	37.774	41.802	1.00 44.86
13									
THE STATE OF THE S	MOTA	502	0	ILE A	66	-16.136	37.735	41.729	1.00 42.69
12 m	MOTA	503	CB	ILE A	66	-14.520	36.947	44.113	1.00 44.28
L.A.	ATOM	504	CG1	ILE A	66	-13.813	37.127	45.445	1.00 47.27
	ATOM	505	CG2	ILE A	66	-14.141	35.578	43.550	1.00 42.84
25	MOTA	506	CD1	ILE A	66	-14.352	36.169	46.514	1.00 38.79
18.5 cm/s	ATOM	507	N	ASN A	67	-14.120	37.549		
un i								40.759	1.00 42.94
}=1,	ATOM	508	CA	ASN A	67	-14.715	37.266	39.472	1.00 44.24
Sec. and	MOTA	509	С	ASN A	67	-15.541	38.444	39.008	1.00 54.25
₩	ATOM	510	0	asn a	67	-16.743	38.344	38.768	1.00 57.56
30	MOTA	511	CB	ASN A	67	-15.595	36.007	39.507	1.00 40.72
T.	MOTA	512	CG	ASN A	67	-14.788	34.759	39.745	1.00 57.39
	ATOM	513		ASN A	67	-13.581	34.711	39.454	
F.									1.00 52.63
	ATOM	514		ASN A	67	-15.446	33.760	40.317	1.00 44.54
(2 H)	ATOM	515	N	GLY A	68	-14.876	39.574	38.899	1.00 50.43
235	ATOM	516	CA	GLY A	68	-15.517	40.796	38.462	1.00 48.89
- A	ATOM	517	С	GLY A	68	-16.807	41.115	39.194	1.00 48.77
	ATOM	518	0	GLY A	68	-17.523	42.018	38.803	1.00 51.39
	ATOM	519	N	GLN A	69	-17.129	40.385	40.244	1.00 40.06
	ATOM		CA						
40		520		GLN A	69	-18.348	40.716	40.928	1.00 40.02
40	ATOM	521	С	GLN A	69	-18.031	41.059	42.364	1.00 50.45
	ATOM	522	0	GLN A	69	-16.943	40.748	42.855	1.00 50.53
	ATOM	523	CB	GLN A	69	-19.415	39.602	40.829	1.00 40.78
	ATOM	524	CG	GLN A	69	-19.966	39.367	39.414	1.00 23.77
	ATOM	525	CD	GLN A	69	-20.513	40.646	38.831	1.00 56.53
45	ATOM	526		GLN A	69	-19.974	41.198		
73								37.859	1.00 55.28
	ATOM	527		GLN A	69	-21.588	41.134	39.437	1.00 62.26
	ATOM	528	N	GLU A	70	-18.975	41.718	43.028	1.00 49.43
	ATOM	529	CA	GLU A	70	-18.766	42.094	44.407	1.00 50.67
	MOTA	530	С	GLU A	70	-19.296	40.996	45.288	1.00 57.90
50	ATOM	531	0	GLU A	70	-20.272	40.367	44.909	1.00 63.90
	ATOM	532	CB	GLU A	70	-19.449	43.434	44.732	1.00 52.26
	ATOM	533	CG	GLU A	70		44.624		
						-18.824		43.970	1.00 64.80
	ATOM	534	CD	GLU A	70	-19.181	45.967	44.555	1.00 91.82
	MOTA	535		GLU A	70	-19.749	46.108	45.629	1.00100.00
55	ATOM	536	OE2	GLU A	70	-18.814	46.963	43.785	1.00 76.01
	ATOM	537	N	VAL A	71	-18.655	40.742	46.433	1.00 47.28
	MOTA	538	CA	VAL A	71	-19.119	39.685	47.335	1.00 43.84
	ATOM	539	С	VAL A	71	-19.434	40.153	48.768	1.00 41.62
/ 0	ATOM	540	0	VAL A	71	-18.983	41.206	49.254	1.00 35.70
60	MOTA	541	CB	VAL A	71	-18.308	38.361	47.273	1.00 46.05
	MOTA	542	CG1	VAL A	71	-18.062	37.923	45.827	1.00 45.19
	MOTA	543		VAL A	71	-16.979	38.460	48.017	1.00 45.24
	ATOM	544	N	LYS A	72	-20.239	39.343	49.431	1.00 39.34
	ATOM	545	CA	LYS A	72	-20.610	39.594	50.792	
	TION	242	CA.	nro W	12	-20.010	33.334	30.132	1.00 42.40

			_			10 047 (F 2 6 6 6	
	MOTA	546	С	LYS A	72		39.466	51.668	1.00 56.92
	MOTA	547	0	LYS A	72	-18.399	38.729	51.334	1.00 59.27
	ATOM	548	CB	LYS A	72	-21.719	38.629	51.211	1.00 45.76
	ATOM	549	CG	LYS A	72		38.960	52.557	1.00 86.98
5									
2	ATOM	550	CD	LYS A	72		38.767	52.606	1.00100.00
	ATOM	551	CE	LYS A	72	-24.656	10.012	53.077	1.00100.00
	MOTA	552	NZ	LYS A	72	-26.011	39.730	53.592	1.00100.00
	ATOM	553	N	TYR A	73	-19.332	40.210	52.780	1.00 55.45
		554	CA	TYR A	73		10.226	53.747	1.00 53.31
10	ATOM								
10	MOTA	555	С	TYR A	73		40.884	55.068	1.00 50.87
	MOTA	556	0	TYR A	73	-19.552	41.703	55.139	1.00 47.82
	MOTA	557	CB	TYR A	73	-16.891	40.741	53.214	1.00 52.73
	MOTA	558	CG	TYR A	73		42.244	53.227	1.00 51.76
		559		TYR A	73		42.946	54.416	
15	MOTA								1.00 52.82
15	MOTA	560		TYR A	73		42.967	52.039	1.00 53.30
	ATOM	561	CE1	TYR A	73	-16.439	44.340	54.422	1.00 52.71
	ATOM	562	CE2	TYR A	73	-16.804	44.359	52.026	1.00 55.39
	ATOM	563	CZ	TYR A	73		45.044	53.229	1.00 63.45
## AA	MOTA	564	OH	TYR A	73		46.404	53.215	1.00 69.53
20	MOTA	565	N	ALA A	74	-17.927	40.494	56.112	1.00 45.37
41	ATOM	566	CA	ALA A	74	-18.180	40.999	57.433	1.00 42.62
	ATOM	567	С	ALA A	74	-16.892	41.265	58.222	1.00 47.81
		568	ō.	ALA A	74		40.554	58.133	
\$=#.	ATOM								1.00 45.50
25	ATOM	569	CB	ALA A	74		40.035	58.170	1.00 40.75
25	ATOM	570	N	LEU A	75	-16.930	42.323	59.005	1.00 49.02
100	ATOM	571	CA	LEU A	75	-15.829	42.693	59.869	1.00 48.85
il.	ATOM	572	С	LEU A	75		42.464	61.281	1.00 47.18
j-k									
lia and	MOTA	573	0	LEU A	75		43.021	61.687	1.00 44.35
*	ATOM	574	CB	LEU A	75		44.136	59.675	1.00 49.64
30	MOTA	575	CG	LEU A	75	-14.789	44.357	58.270	1.00 58.09
er	MOTA	576	CD1	LEU A	75	-14.524	45.841	58.023	1.00 61.34
	MOTA	577		LEU A	75		43.565	58.069	1.00 62.34
2 pt/	MOTA	578	N	GLY A	76		41.592	62.004	1.00 47.67
La	MOTA	579	CA	GLY A	76	-16.034	41.281	63.359	1.00 46.79
35	MOTA	580	С	GLY A	76	-15.495	42.337	64.279	1.00 47.74
is in	ATOM	581	0	GLY A	76		43.171	63.882	1.00 42.87
Az ez		582	N	GLU A	77		42.311	65.502	
	ATOM								1.00 48.32
	MOTA	583	CA	GLU A	77		43.300	66.431	1.00 52.14
	ATOM	584	С	GLU A	77	-14.029	43.195	66.679	1.00 56.71
40	ATOM	585	0	GLU A	77	-13.418	42.120	66.591	1.00 55.78
	ATOM	586	CB	GLU A	77	-16.357	43.341	67.732	1.00 55.55
	ATOM	587	CG	GLU A	77		42.063	67.969	1.00 79.57
	ATOM	588	CD	GLU A	77		41.739	69.427	1.00100.00
	ATOM	589		GLU A	77	-16.537	41.435	70.211	1.00100.00
45	ATOM	590	OE2	GLU A	77	-18.712	41.799	69.770	1.00100.00
	ATOM	591	N	ARG A	78	-13.452	44.344	67.000	1.00 54.17
	ATOM	592	CA	ARG A	78		44.433	67.298	1.00 53.38
	ATOM	593	С	ARG A	78		43.656	68.579	1.00 58.88
	ATOM	594	0	ARG A	78	-12.247	43.767	69.635	1.00 61.35
50	MOTA	595	CB	ARG A	78	-11.571	45.891	67.367	1.00 41.96
	MOTA	596	CG	ARG A	78	-10.050	46.006	67.326	1.00 38.20
		597	CD		78				
	MOTA			ARG A			47.411	67.551	1.00 44.73
	ATOM	598	NE	ARG A	78		47.648	66.842	1.00 66.47
	MOTA	599	CZ	ARG A	78	-7.250	48.247	67.389	1.00 97.61
55	ATOM	600	NH1	ARG A	78	-7.276	48.692	68.645	1.00100.00
	ATOM	601		ARG A	78		48.413	66.663	1.00 80.10
	ATOM	602	N	GLN A	79		42.857	68.463	1.00 49.54
	MOTA	603	CA	GLN A	79		42.115	69.566	1.00 47.71
	ATOM	604	С	GLN A	79	-8.664	42.789	69.865	1.00 49.77
60	ATOM	605	0	GLN A	79		42.421	69.333	1.00 52.63
	ATOM	606	CB	GLN A	79		40.613	69.240	1.00 49.05
	ATOM	607	CG	GLN A	79		39.794	69.339	1.00 57.32
	ATOM	608	CD	GLN A	79		38.435	68.656	1.00 69.51
	ATOM	609	OE1	GLN A	79	-10.400	37.480	69.152	1.00 49.72
	* £ _				-				

	ATOM	610	NE2	GLN A	79	-11.727	38.340	67.517	1 00	62.60
	ATOM	611	N	SER A	80	-8.699	43.826	70.683		
	ATOM	612	CA	SER A						41.74
					80	-7.490	44.543	71.022		37.90
_	ATOM	613	С	SER A	80	-6.437	44.559	69.920	1.00	35.98
, 5	ATOM	614	0	SER A	80	-6.736	44.939	68.801	1.00	34.52
	ATOM	615	CB	SER A	80	-6.910	44.144	72.372		39.07
	ATOM	616	OG	SER A	80	-7.255	42.803	72.684		61.32
	ATOM	617	N	TYR A	81	-5.206				
			CA				44.154	70.289		29.92
10	ATOM	618		TYR A	81	-4.027	44.114	69.430		26.45
10	MOTA	619	С	TYR A	81	-4.163	43.116	68.285	1.00	30.82
	ATOM	620	0	TYR A	81	-3.480	43.215	67.269		34.48
	ATOM	621	CB	TYR A	81	-2.727	43.893	70.257		25.19
	ATOM	622	CG	TYR A	81	-2.713				
	ATOM	623		TYR A			42.491	70.839		24.57
15					81	-3.327	42.247	72.066	1.00	27.27
15	ATOM	624		TYR A	81	-2.165	41.410	70.148	1.00	21.82
	ATOM	625	CE1	TYR A	81	-3.380	40.975	72.632	1.00	26.49
	ATOM	626	CE2	TYR A	81	-2.230	40.122	70.682	1 00	23.48
	MOTA	627	CZ	TYR A	81	-2.827	39.908	71.930		
	ATOM	628	OH	TYR A						38.28
					81	-2.889	38.653	72.493		42.17
20	ATOM	629	N	LYS A	82	-5.038	42.136	68.415	1.00	26.97
d)	MOTA	630	CA	LYS A	82	-5.170	41.229	67.293	1.00	27.99
ja š.	MOTA	631	С	LYS A	82	-5.867	41.898	66.072		38.90
	MOTA	632	0	LYS A	82	-5.614	41.541	64.900		
100	ATOM	633	СВ	LYS A	82					37.15
25						-5.785	39.918	67.708		27.59
25	ATOM	634	CG	LYS A	82	-5.169	39.451	69.008	1.00	39.68
	ATOM	635	CD	LYS A	82	-5.435	37.993	69.350	1.00	46.78
J=6.	ATOM	636	CE	LYS A	82	-6.414	37.819	70.492		59.84
	ATOM	637	NZ	LYS A	82	-7.097	36.523	70.452		63.48
	ATOM	638	N	GLY A	83	-6.738				
30	- ATOM	639	CA				42.894	66.367		35.64
T. 30				GLY A	83	-7.512	43.620	65.368		33.65
	MOTA	640	С	GLY A	83	-8.866	42.925	65.111	1.00	32.95
1 . m.	ATOM	641	0	GLY A	83	-9.297	42.063	65.870	1.00	28.28
17	ATOM	642	N	SER A	84	-9.535	43.300	64.026		34.51
35	ATOM	643	CA	SER A	84	-10.839	42.742	63.673		36.13
35	ATOM	644	С	SER A	84	-10.796				
3,44	ATOM	645	Ö				41.724	62.549		40.65
				SER A	84	-10.173	41.893	61.501		39.77
	ATOM	646	CB	SER A	84	-11.883	43.808	63.383	1.00	37.68
	ATOM	647	OG	SER A	84	-11.812	44.832	64.352	1.00	45.14
	ATOM	648	N	PRO A	85	-11.491	40.656	62.791		37.01
40	ATOM	649	CA	PRO A	85	-11.573	39.559	61.863		34.91
	ATOM	650	С	PRO A	85	-12.459	39.946			
	ATOM	651	ŏ	PRO A	85			60.712	1.00	
						-13.514	40.522	60.941		35.30
	ATOM	652	CB	PRO A	85	-12.227	38.406	62.647	1.00	
4.5	ATOM	653	CG	PRO A	85	-12.714	38.981	63.974	1.00	44.97
45	MOTA	654	CD	PRO A	85	-12.325	40.462	64.004	1.00	
	ATOM	655	N	MET A	86	-12.018	39.642	59.487	1.00	
	ATOM	656	CA	MET A	86	-12.756	39.960	58.275	1.00	
	ATOM	657	С	MET A	86	-13.165				
	MOTA						38.683	57.552	1.00	
50		658	0	MET A	86	-12.338	38.015	56.954	1.00	
30	MOTA	659	CB	MET A	86	-11.921	40.829	57.337	1.00	29.51
	MOTA	660	CG	MET A	86	-12.750	41.242	56.136	1.00	
	ATOM	661	SD	MET A	86	-11.816	41.878	54.701	1.00	
	ATOM	662	CE	MET A	86	-13.244	42.527			
	ATOM	663	N	GLU A	87			53.805	1.00	
55						-14.441	38.324	57.610	1.00	
33	ATOM	664	CA	GLU A	87	-14.912	37.107	56.950	1.00	
	ATOM	665	С	GLU A	87	-15.495	37.352	55.560	1.00	51.53
	ATOM	666	0	GLU A	87	-16.425	38.129	55.424	1.00	
	ATOM	667	CB	GLU A	87	-15.942	36.390	57.813	1.00	
	ATOM	668	CG	GLU A	87	-16.144				
60	ATOM	669	CD	GLU A	87		34.937	57.389	1.00	
						-17.300	34.316	58.104	1.00	
	ATOM	670		GLU A	87	-18.439	34.738	57.994	1.00	
	MOTA	671	OE2		87	-16.943	33.301	58.868	1.00	
	ATOM	672	N	ILE A	88	-14.942	36.659	54.544	1.00	
	ATOM	673	CA	ILE A	88	-15.332	36.765	53.145	1.00	

	ATOM	674	С	ILE A	88	-16.14	15 35.610	52.613	1 00 46 70
	ATOM	675	Ö	ILE A	88	-15.72		52.656	1.00 46.72 1.00 48.10
	ATOM	676	СB	ILE A	88	-14.10		52.292	1.00 48.10
	ATOM	677		ILE A	88	-13.3	-	52.696	1.00 39.13
5	ATOM	678			88	-14.5		50.839	1.00 28.13
	ATOM	679		ILE A	88	-11.9		52.051	1.00 20.13
	ATOM	680	N	SER A	89	-17.3		52.077	1.00 45.16
	ATOM	681	CA	SER A	89	-18.1		51.559	1.00 44.76
	ATOM	682	С	SER A	89	-17.90		50.131	1.00 46.01
10	ATOM	683	0	SER A	89	-18.04		49.243	1.00 44.34
	MOTA	684	CB	SER A	89	-19.6	35.121	51.827	1.00 51.87
	ATOM	685	OG	SER A	89	-19.94		53.198	1.00 69.07
	MOTA	686	N	LEU A	90	-17.49	33.279	49.914	1.00 46.43
	MOTA	687	CA	LEU A	90	-17.20		48.575	1.00 46.93
15	ATOM	688	C	LEU A	90	-18.4		47.935	1.00 55.26
	ATOM	689	0	LEU A	90	-19.2		48.556	1.00 54.94
	ATOM	690	CB	LEU A	90	-16.08		48.521	1.00 46.14
100 mg	ATOM	691	CG	LEU A	90	-15.26		49.792	1.00 50.78
	ATOM	692		LEU A	90	-14.54		49.806	1.00 50.27
20	ATOM	693		LEU A	90	-14.2		49.863	1.00 55.52
j.k	ATOM	694	N	PRO A	91	-18.62		46.683	1.00 54.81
	ATOM	695	CA	PRO A	91	-19.75		45.870	1.00 58.45
g sile unig max sumo	ATOM	696	c	PRO A	91	-19.58		45.254	1.00 67.78
25	ATOM ATOM	697 698	O CB	PRO A	91	-20.50		44.623	1.00 68.64
	ATOM	699	CG	PRO A	91	-19.84		44.738	1.00 59.70
*	ATOM	700	CD	PRO A	91 91	-18.50		44.711	1.00 61.25
	ATOM	701	N	ILE A	92	-17.73 -18.41		45.961	1.00 54.16
j.	ATOM	702	CA	ILE A	92	-18.23		45.416 44.850	1.00 64.82
30	ATOM	703	c	ILE A	92	-17.48		45.801	1.00 65.03 1.00 66.34
	ATOM	704	o	ILE A	92	-16.2		45.865	1.00 70.20
	ATOM	705	CB	ILE A	92	-17.43		43.547	1.00 70.20
22 mg	ATOM	706	CG1	ILE A	92	-18.29		42.430	1.00 70.02
	ATOM	707		ILE A	92	-16.9		43.171	1.00 71.86
- 35	MOTA	708	CD1	ILE A	92	-17.52		41.121	1.00 80.63
	ATOM	709	N	ALA A	93	-18.23	9 27.115	46.534	1.00 54.40
	ATOM	710	CA	ALA A	93	-17.52	26.247	47.452	1.00 51.74
	MOTA	711	С	ALA A	93	-16.26		46.804	1.00 52.66
40	ATOM	712	0	ALA A	93	-16.28		45.662	1.00 49.87
40	ATOM	713	CB	ALA A	93	-18.36		47.968	1.00 52.76
	ATOM	714	N	LEU A	94	-15.16		47.544	1.00 48.18
	ATOM ATOM	715	CA	LEU A	94	-13.86		47.067	1.00 43.27
	ATOM	716 717	C O	LEU A	94	-13.56		47.581	1.00 43.98
45	ATOM	718	СВ	LEU A	94 94	-14.08		48.601	1.00 44.63
	ATOM	719	CG	LEU A	94	-12.71 -12.68		47.509	1.00 41.05
	ATOM	720		LEU A	94	-11.27	35 27.638 72 28.200	46.739	1.00 40.03
	ATOM	721		LEU A	94	-13.11		46.751 45.311	1.00 36.88 1.00 44.98
	ATOM	722	N	SER A	95	-12.70		46.875	1.00 44.98
50	ATOM	723	CA	SER A	95	-12.32		47.256	1.00 43.26
	ATOM	724	C	SER A	95	-10.80		47.344	1.00 38.58
	ATOM	725	0	SER A	95	-10.08		46.975	1.00 36.78
	ATOM	726	CB	SER A	95	-12.90		46.256	1.00 51.55
	ATOM	727	OG	SER A	95	-14.29		46.156	1.00 62.74
55	ATOM	728	N	LYS A	96	-10.32		47.830	1.00 31.10
	ATOM	729	CA	LYS A	96	-8.88		47.958	1.00 34.92
	ATOM	730	С	LYS A	96	-8.05	8 21.238	46.777	1.00 45.63
	ATOM	731	0	LYS A	96	-8.40		45.612	1.00 49.35
60	ATOM	732	CB	LYS A	96	-8.40		48.451	1.00 38.53
60	ATOM	733	CG	LYS A	96	-9.18		49.651	1.00 68.97
	ATOM	734	CD	LYS A	96	-8.69		50.221	1.00 80.86
	ATOM	735	CE	LYS A	96	-9.59		51.330	1.00 92.53
	ATOM	736	NZ	LYS A	96	-9.04		52.029	1.00100.00
	ATOM	737	N	ASN A	97	-6.94	21.873	47.108	1.00 41.92

	MOTA	738	CA	ASN A	97	-6.009	22.403	46.139	3 00	40.91
	MOTA	739	С	ASN A		-6.606	23.348	45.088		42.64
	ATOM	740	0	ASN A		-5.963	23.681	44.068		38.69
	ATOM	741	CB	ASN A		-5.084	21.304	45.583		28.16
5	ATOM	742	CG	ASN A		-4.327	20.568	46.677		52.21
	ATOM	743		ASN A		-3.089	20.627	46.744		
	ATOM	744	ND2			-5.060	19.858	47.533		55.30
	ATOM	745	N	GLN A		-7.833				53.87
	ATOM	746	CA	GLN A			23.791	45.382		36.59
10	ATOM	747	C	GLN A		-8.557	24.718	44.536		38.44
, 10	ATOM	748				-8.288	26.181	44.951		43.30
	ATOM		0	GLN A		-8.248	26.526	46.138		43.40
		749	CB	GLN A		-10.064	24.395	44.575		42.26
	ATOM	750	CG	GLN A		-10.553	23.538	43.385		68.24
15	ATOM	751	CD	GLN A		-12.008	23.778	43.010		95.57
15	ATOM	752	OE1	GLN A		-12.890	22.935	43.278	1.00	86.92
	ATOM	753	NE2	GLN A		-12.271	24.935	42.393	1.00	95.48
	ATOM	754	N	GLU A		-8.089	27.062	43.973	1.00	39.70
120 St.	MOTA	755	CA	GLU A	99	-7.817	28.468	44.280	1.00	40.49
20	ATOM	756	С	GLU A	99	-8.750	29.536	43.683		47.84
20	MOTA	757	0	GLU A	99	-9.330	29.394	42.606		46.85
	ATOM	758	CB	GLU A	99	-6.361	28.866	43.951		40.24
1=4 ₀	ATOM	759	CG	GLU A	99	-5.608	27.861	43.080		44.16
\$ 710. 1 110.	ATOM	760	CD	GLU A	99	-4.120	28.119	42.990		
\$ \$700, (10) 400	ATOM	761	OE1	GLU A	99	-3.636	29.062	42.376		73.95
25	ATOM	762	OE2	GLU A	99	-3.395	27.210	43.614		55.99
ga A.	ATOM	763	N	ILE A		-8.848	30.643	44.418		43.55
	ATOM	764	CA	ILE A		-9.595	31.800	44.005		43.46
## ·	ATOM	765	С	ILE A		-8.701	32.992	44.238		
jst.	ATOM	766	ō	ILE A		-7.725	32.927	45.004		53.31
30	ATOM	767	СВ	ILE A		-10.881	32.068	44.773		55.16
	ATOM	768	CG1	ILE A		-10.762	31.640			46.65
	ATOM	769	CG2	ILE A		-12.111		46.227		50.76
स्य का मुंदर का	ATOM	770		ILE A			31.486	44.106		46.76
	ATOM	771	N	VAL A		-9.959	32.620	47.087		64.36
35	ATOM	772	CA	VAL A		-9.060	34.076	43.580		48.20
	ATOM	773	CA	VAL A		-8.382	35.329	43.760		45.63
	ATOM	774	0			-9.383	36.351			48.59
	ATOM	775	CB	VAL A		-10.331	36.722	43.623		51.29
	ATOM	776				-7.461	35.793	42.633		45.06
40	ATOM		CG1	VAL A		-7.693	35.000	41.378		43.25
70		777	CG2	VAL A		-7.609	37.289	42.395		45.02
	ATOM ATOM	778	N	ILE A		-9.182	36.738	45.546		41.15
		779	CA	ILE A		-10.023	37.690	46.238		39.43
	MOTA	780	C	ILE A		-9.439	39.062	46.170		49.35
45	ATOM	781	0	ILE A		-8.331	39.274	46.659		53.80
43	ATOM	782	CB	ILE A		-10.097	37.319	47.694	1.00	39.19
	ATOM	783	CGT	ILE A	102	-10.180	35.800	47.809		35.28
	ATOM	784		ILE A		-11.300	37.992	48.341		35.25
	ATOM	785		ILE A		-10.962	35.392	49.044	1.00	47.09
50	ATOM	786	N	GLU A		-10.192	39.984	45.572		43.20
30	MOTA	787	CA	GLU A		-9.748	41.362	45.433		39.88
	ATOM	788	С	GLU A		-10.378	42.299	46.425	1.00	44.03
	MOTA	789	0	GLU A		-11.580	42.558	46.385	1.00	41.34
	MOTA	790	CB	GLU A		-9.950	41.930	44.047		39.11
	ATOM	791	CG	GLU A		-9.017	43.112	43.863	1.00	36.18
55	ATOM	792	CD	GLU A		-9.150	43.666	42.485		61.93
	ATOM	793	OE1	GLU A		-10.157	44.234	42.100		69.89
	ATOM	794	OE2			-8.087	43.457	41.744		76.18
	MOTA	795	N	ILE A		-9.534	42.797	47.322		42.69
	ATOM	796	CA	ILE A		-9.969	43.718	48.346		40.72
60	ATOM	797	С	ILE A		-9.522	45.167	48.099		46.21
	ATOM	798	o	ILE A		-8.346	45.478	47.866		40.21
	ATOM	799	СВ	ILE A		-9.578	43.283	49.754		42.68
	ATOM	800		ILE A		-10.006	41.855	50.032		
	ATOM	801	CG2	ILE A	104	-10.225				39.85
				~ A	- 07	10.223	44.222	50.768	T • OO	41.53

	. A'	TOM	802	CD1	ILE	Α	104	-8.839	40.99	35	50.485	1 00	34.17
	Δ.	TOM	803	N	SER			-10.506	46.05		48.173		
		TOM	804	CA	SER								47.94
								-10.278	47.48		48.046		48.05
_	A'	TOM	805	С	SER	Α	105	-10.184	47.97	17	49.482	1.00	42.39
5	A'	TOM	806	0	SER	Α	105	-11.134	47.87	79	50.263		39.69
	A'	TOM	807	CB	SER			-11.399	48.18		47.290		
		TOM	808	OG									53.77
					SER			-11.399	47.78		45.930		60.69
		TOM	809	N	PHE			-9.020	48.44	15	49.857	1.00	35.07
	A'	TOM	810	ÇA	PHE	Α	106	-8.844	48.89	0	51.223	1.00	34.98
10	A'	TOM	811	С	PHE	Α	106	-8.177	50.23		51.262		39.26
		TOM	812	0	PHE			-7.607	50.73				
											50.265		34.24
		TOM	813	CB	PHE			-8.015	47.86		52.060	1.00	36.05
	A'	TOM	814	CG	PHE	A	106	-6.581	47.81	.5	51.556	1.00	37.24
	A'	TOM	815	CD1	PHE	Α	106	-6.251	47.07		50.422		39.71
15	A ⁴	TOM	816		PHE			-5.579	48.57		52.161		
			817		PHE								36.44
		TOM						-4.950	47.08		49.920		41.48
		TOM	818		PHE	A	106	-4.273	48.60	9 .	51.672	1.00	38.19
	A'	TOM	819	CZ	PHE	Α	106	-3.961	47.85	6	50.540		37.91
संस्था करते । अस्त्राच्या	A'	TOM	820	N	GLU	Α	107	-8.284	50.79		52.453		40.64
20		TOM	821	CA	GLU			-7.711					
20									52.06		52.848		43.81
-		TOM	822	С	GLU			-7.206	51.86		54.284	1.00	43.82
	A'	TOM	823	0	GLU	Α	107	-7.933	51.30	3	55.121	1.00	38.38
ad as	A'	TOM	824	CB	GLU	Α	107	-8.737	53.23		52.753		46.93
##\	A'	TOM	825	CG	GLU	Δ	107	-8.107	54.63		52.467		
25		TOM	826	CD	GLU								67.21
- 20								-9.086	55.71		52.042		100.00
In La		TOM	827	OE1	GLU			-10.208	55.50		51.599	1.00	100.00
ies.	A'	TOM	828	OE2	GLU	Α	107	-8.631	56.93	8	52.221		93.72
**	A'	TOM	829	N	THR	Α	108	-5.963	52.29		54.551		39.12
₩#.	A'	TOM	830	CA	THR			-5.345	52.17		55.873		
30		TOM	831	С									39.69
					THR			-5.564	53.42		56.724		49.82
R Tage		TOM	832	0	THR			-5.565	54.55	2	56.177	1.00	50.94
122 224 122 227		TOM	833	CB	THR			-3.810	52.09	5 !	55.722	1.00	40.40
	A.	TOM	834	OG1	THR	A	108	-3.360	53.22	6	54.981	1.00	32.22
11 5	A'	TOM	835	CG2	THR .	Α	108	-3.371	50.80		55.042		46.43
35	A'	TOM	836	N	SER .			-5.698	53.21		58.065		
		TOM	837	CA	SER								42.02
								-5.848	54.29		59.038		38.13
		TOM	838	С	SER .			-4.555	55.10	1 :	59.082	1.00	38.47
	A:	TOM	839	0	SER .	Ą	109	-3.460	54.58	3 !	58.921	1.00	33.60
	A'	TOM	840	CB	SER .	A	109	-6.166	53.75	9 (50.437		41.44
40	A'	TOM	841	OG	SER .			-6.205	54.81		51.404		47.63
		TOM	842	N	PRO .								
		TOM						-4.655	56.39		59.308		41.64
			843	CA	PRO .			-3.419	57.11		59.393	1.00	40.75
	A:	TOM	844	С	PRO .	A	110	-2.803	56.74	9 (50.725	1.00	41.47
	A'	TOM	845	0	PRO .	A	110	-1.676	57.08		61.009	1.00	42.30
45	A.	TOM	846	CB	PRO .	Α	110	-3.721	58.60		59.298		42.09
	Αr	TOM	847	CG	PRO .								
		TOM	848	CD				-5.224	58.71		59.132		48.77
					PRO .			-5.811	57.31		59.269	1.00	44.58
	A:	TOM	849	N	LYS .			-3.578	56.01	7 6	51.518	1.00	36.35
	A.	TOM	850	CA	LYS .	Α	111	-3.167	55.53		52.819		36.74
50	A.	TOM	851		LYS .			-2.669	54.08		52.720		40.19
		TOM	852		LYS .								
		TOM	853					-2.733	53.31		53.678		40.53
					LYS .			-4.341	55.60	6 6	53.807	1.00	41.91
		FOM	854		LYS .			-4.362	56.83	8 6	54.708	1.00	71.21
	A.	TOM	855	CD	LYS .	A	111	-5.421	57.85		54.309		97.95
55	A.	TOM	856		LYS .			-6.839	57.39				
		rom	857								54.611		100.00
					LYS .			-7.853	58.12		53.819	1.003	100.00
		rom	858	N	SER .			-2.184	53.67	0 €	51.550	1.00	36.84
	A.	TOM	859	CA	SER .	A	112	-1.714	52.29		51.358		34.35
100	A.	rom	860		SER .			-0.518	51.91		52.225		35.57
60		rom	861		SER			0.533	52.54				
,		rom	862		SER I						52.166		32.49
								-1.449	51.99		9.883		35.16
		rom Tox	863		SER I			-0.682	50.81		9.762	1.00	31.94
		TOM		N	SER A	A	113	-0.666	50.87	2 6	53.033		31.84
	A.	TOM	865	CA	SER .	A	113	0.445	50.46		3.866		29.27
							0		• 10	•			

	MOTA	866	С	SER			1.601	49.927	63.040	1.00	33.37
	MOTA	867	0	SER			2.715	49.792	63.497	1.00	32.95
	MOTA	868	CB	SER			0.052	49.498	64.945		29.45
_	MOTA	869	OG	SER			0.045	48.169	64.462	1.00	34.27
5	ATOM	870	N	ALA			1.357	49.628	61.797	1.00	33.69
	ATOM	871	CA	ALA			2.437	49.134	60.981		34.05
	ATOM	872	С	ALA			3.239	50.287	60.388		37.83
	ATOM	873	0	ALA			4.411	50.149	60.033		37.72
10	ATOM	874	CB	ALA			1.845	48.292	59.852		34.51
10	ATOM	875 876	N CA	LEU			2.580	51.432	60.259		32.19
	ATOM ATOM	877	CA	LEU LEU			3.201	52.595	59.662		30.48
	ATOM	878	0	LEU			3.509	53.745	60.565		35.32
	ATOM	879	CB	LEU			2.902 2.358	54.012	61.604		35.25
15	ATOM	880	CG	LEU			1.787	53.156 52.064	58.507 57.602		30.53
13	ATOM	881		LEU			0.812	52.710	56.637		35.51
	ATOM	882		LEU			2.903	51.387	56.821		35.12
	ATOM	883	N	GLN			4.490	54.457	60.096		33.88 34.00
	ATOM	884	CA	GLN			4.926	55.656	60.737		32.52
20	MOTA	885	c	GLN			5.066	56.689	59.645		31.34
in it was	ATOM	886	ō	GLN			5.880	56.552-			28.29
j=4,	ATOM	887	СВ	GLN			6.232	55.540	61.496		32.66
1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	ATOM	888	CG	GLN			6.419	56.813	62.322		41.25
1 mm/	ATOM	889	CD	GLN			7.777	56.897	62.952		50.08
25	ATOM	890		GLN			8.515	55.905	63.017		55.36
### 12°	ATOM	891		GLN			8.090	58.081	63.438		38.23
	MOTA	892	N	TRP			4.210	57.680	59.748		26.66
盘	ATOM	893	CA	TRP	Α	117	4.148	58.785	58.827		26.04
haba	MOTA	894	C	TRP	Α	117	4.912	59.978	59.375		34.56
1. 30	ATOM	895	0	TRP	Α	117	4.467	60.589	60.364		36.83
T.	ATOM	896	CB	TRP			2.669	59.188	58.630		23.15
14.1	MOTA	897	CG	TRP			1.826	58.209	57.863	1.00	23.02
11	ATOM	898		TRP			1.052	57.224	58.397	1.00	26.39
	ATOM	899		TRP			1.640	58.135	56.433	1.00	21.06
≯ 35 ्	ATOM	900		TRP			0.395	56.534	57.393	1.00	26.40
	ATOM	901		TRP			0.735	57.087	56.184	1.00	27.99
	ATOM	902		TRP			2.121	58.872	55.361		20.95
	ATOM	903		TRP			0.352	56.753	54.886		28.21
40	ATOM ATOM	904 905	CZ3	TRP TRP			1.750	58.560	54.079		22.43
40	ATOM	906	N N	LEU			0.872 6.043	57.512	53,847		24.28
	ATOM	907	CA	LEU			6.745	60.340 61.506	58.756		31.44
	ATOM	908	C	LEU			6.584	62.774	59.276 58.432		36.67 46.93
	ATOM	909	ō	LEU			6.434	62.705	57.210		51.17
45	ATOM	910	СВ	LEU			8.250	61.327	59.577		38.83
	ATOM	911	CG	LEU			8.881	59.939	59.398		44.33
	ATOM	912	CD1	LEU	Α	118	10.392	60.065	59.569		42.12
	MOTA	913		LEU			8.351	58.950	60.426		49.99
	ATOM	914	N	THR			6.524	63.939	59.109		41.34
50	ATOM	915	CA	THR	A	119	6.449	65.260	58.468		38.89
	ATOM	916	С	THR			7.847	65.633	58.034		40.14
	ATOM	917	0	THR			8.841	65.165	58.605		44.03
	ATOM	918	CB	THR			5.932	66.300	59.467		42.63
	ATOM	919		THR	Α	119	6.994	66.605	60.362	1.00	50.01
55	ATOM	920	CG2				4.769	65.668	60.224		36.78
	MOTA	921	N	PRO			7.963	66.440	57.020	1.00	33.41
	ATOM	922	CA	PRO			9.275	66.781	56.517	1.00	33.18
	ATOM	923	C	PRO			10.260	67.209	57.599	1.00	38.27
60	ATOM	924	0	PRO			11.433	66.829	57.566		34.42
UU	ATOM	925	CB	PRO			9.068	67.840	55.416		33.54
	ATOM	926	CG	PRO			7.582	67.823	55.097		34.86
	ATOM ATOM	927 928	CD N	PRO			6.891	67.180	56.300		30.86
	ATOM	929	CA	GLU			9.751	67.982	58.563		38.03
	AION	263	~∧	GTO	Α.	121	10.534	68.474	59.681	1.00	41.03

	ATOM	930	С	GLU A 121	<u>l</u>	11.212	67.361	60.411	1.00 50.88
	ATOM	931	0	GLU A 121	ì	12.279	67.548	60.977	
	ATOM	932	СВ						1.00 54.97
				GLU A 121		9.742	69.325	60.699	1.00 43.28
	ATOM	933	CG	GLU A 121	L	8.220	69.071	60.702	1.00 64.72
5	ATOM	934	CD	GLU A 121		7.398	70.118	59.988	1.00 86.07
	ATOM	935	OE1						
						7.007	71.131	60.538	1.00100.00
	ATOM	936	OE2	GLU A 121	,	7.108	69.803	58.739	1.00 59.72
	ATOM	937	N	GLN A 122	2	10.569	66.202	60.394	1.00 44.09
	ATOM	938	CA	GLN A 122	>	11.083	65.019	61.041	
10	ATOM	939	c	GLN A 122					1.00 40.20
10						12.170	64.373	60.232	1.00 47.73
	ATOM	940	0	GLN A 122	?	12.711	63.343	60.643	1.00 53.29
	ATOM	941	CB	GLN A 122	2	9.965	63.992	61.224	1.00 39.31
	ATOM	942	CG	GLN A 122	•	9.057	64.441	62.361	
	ATOM	943	CD	GLN A 122					1.00 30.23
15						7.756	63.691	62.438	1.00 38.25
13	MOTA	944	OE1		2	6.899	63.804	61.548	1.00 53.34
	ATOM	945	NE2	GLN A 122	?	7.592	62.938	63.521	1.00 18.98
	MOTA	946	N	THR A 123		12.486	64.942		
art on	ATOM	947	CA					59.074	1.00 38.99
				THR A 123		13.490	64.319	58.229	1.00 36.00
1. 1 ⁵⁸ 1	ATOM	948	С	THR A 123	3	14.755	65.034	58.264	1.00 35.30
20	ATOM	949	0	THR A 123	3	14.842	66.074	58.875	1.00 34.95
13	MOTA	950	CB	THR A 123					
\$=#x						13.067	64.145	56.759	1.00 38.25
	MOTA	951	OG1			13.144	65.374	56.046	1.00 43.75
	ATOM	952	CG2	THR A 123	3	11.643	63.616	56.725	1.00 40.72
2 550	ATOM	953	N	SER A 124	l	15.699	64.447	57.557	
25	ATOM	954	CA	SER A 124		17.025			1.00 32.18
25							64.996	57.442	1.00 33.71
\$=5.	ATOM	955	С	SER A 124		17.007	66.216	56.553	1.00 39.04
1	ATOM	956	0	SER A 124	l	17.537	67.268	56.883	1.00 39.07
運	ATOM	957	CB	SER A 124		18.023	63.992	56.859	
la flo	ATOM	958	OG						1.00 37.73
30				SER A 124		18.359	62.978	57.796	1.00 36.28
	MOTA	959	N	GLY A 125		16.389	66.025	55.414	1.00 38.59
T.	ATOM	960	CA	GLY A 125)	16.280	67.034	54.396	1.00 39.90
	MOTA	961	С	GLY A 125		15.290	68.094		
in and	ATOM	962						54.749	1.00 46.83
			0	GLY A 125		15.347	69.171	54.172	1.00 49.78
	ATOM	963	N	LYS A 126		14.391	67.788	55.678	1.00 41.09
35	ATOM	964	CA	LYS A 126	;	13.396	68.761	56.126	1.00 41.26
	ATOM	965	С	LYS A 126		12.498	69.307	55.020	
	ATOM	966	Ö						1.00 47.42
				LYS A 126		11.617	70.141	55.279	1.00 48.94
	ATOM	967	СВ	LYS A 126		14.024	69.936	56.894	1.00 41.98
	ATOM	968	CG	LYS A 126	;	15.094	69.555	57.913	1.00 45.84
40	ATOM	969	CD	LYS A 126	i	14.535	68.838	59.135	1.00 58.74
	ATOM	970	CE	LYS A 126					
						15.612	68.500	60.151	1.00 72.12
4	ATOM	971	NZ	LYS A 126		15.395	67.218	60.839	1.00 88.38
	MOTA	972	N	GLU A 127	'	12.722	68.858	53.792	1.00 41.82
	ATOM	973	CA	GLU A 127	•	11.921	69.344	52.708	1.00 41.98
45	ATOM	974	C	GLU A 127		10.899	68.334		
								52.239	1.00 45.14
	ATOM	975	0	GLU A 127		9.994	68.683	51.496	1.00 46.95
	ATOM	976	CB	GLU A 127		12.727	70.015	51.543	1.00 44.39
	ATOM	977	CG	GLU A 127	•	13.198	71.499	51.820	1.00 57.99
	ATOM	978	CD	GLU A 127		12.331	72.659	51.301	
50	ATOM	979		GLU A 127				21.201	1.00100.00
20						11.652	72.611	50.286	1.00100.00
	ATOM	980	OE2	GLU A 127		12.387	73.758	52.054	1.00100.00
	ATOM	981	N	HIS A 128	:	11.027	67.077	52.653	1.00 39.18
	ATOM	982	CA	HIS A 128		10.068			
	ATOM	983					66.072	52.210	1.00 39.43
55			С	HIS A 128		9.636	65.148	53.316	1.00 42.09
دد	ATOM	984	0	HIS A 128		10.366	64.955	54.281	1.00 45.34
	ATOM	985	CB	HIS A 128		10.628	65.194	51.097	1.00 42.16
	MOTA	986	CG	HIS A 128		10.947	65.936		
								49.854	1.00 47.24
	ATOM	987		HIS A 128		9.943	66.423	49.029	1.00 49.12
	ATOM	988		HIS A 128		12.159	66.262	49.322	1.00 51.13
60	ATOM	989	CEl	HIS A 128		10.559	67.031	48.026	1.00 49.97
	ATOM	990		HIS A 128		11.888	66.953	48.166	
	MOTA	991							1.00 50.87
			N	PRO A 129		8.447	64.572	53.171	1.00 32.55
	ATOM	992	CA	PRO A 129		7.968	63.650	54.163	1.00 31.15
	ATOM	993	С	PRO A 129		8.636	62.328	53.900	1.00 34.90
									00 04.50

	MOTA	994	0	PRO A 1	L29	9.481	62.214	53.021	1.00	35.46
	MOTA	995	CB	PRO A 1	129	6.466	63.490	53.986		31.94
	MOTA	996	CG	PRO A 1	129	6.133	64.104	52.649		36.83
	MOTA	997	CD	PRO A 1	L29	7.384	64.850	52.185		
5	ATOM	998	N	TYR A 1	130	8.248	61.342	54.659		29.47
	MOTA	999	CA	TYR A 1		8.826	60.025	54.548		29.35
	MOTA	1000	C	TYR A 1		7.856	59.046	55.156		31.83
	ATOM	1001	0	TYR A 1	130	7.138	59.375	56.093		29.84
	ATOM	1002	CB	TYR A 1		10.098	60.029	55.433		30.54
10	ATOM	1003	CG	TYR A 1		11.083	58.886	55.285		29.76
	ATOM	1004	CD1	TYR A 1	130	10.845	57.630	55.845		26.16
	ATOM	1005	CD2			12.290	59.110	54.619		30.28
	MOTA	1006	CE1	TYR A 1		11.795	56.621	55.721		17.87
4	MOTA	1007	CE2			13.253	58.114	54.479		27.75
15	MOTA	1008	CZ	TYR A 1		12.983	56.866	55.031		25.76
	ATOM	1009	ОН	TYR A 1		13.899	55.864	54.894		40.52
	ATOM	1010	N	LEU A 1		7.832	57.842	54.647		31.12
	ATOM	1011	CA	LEU A 1		6.994	56.868	55.303		
200 EE	ATOM	1012	C	LEU A 1		7.691	55.568	55.289		30.43
20	ATOM	1013	Ö	LEU A 1		8.398	55.257			33.91
	ATOM	1014	CB	LEU A 1		5.679		54.397		33.68
	ATOM	1015	CG	LEU A 1		5.065	56.761	54.530		26.16
jado.	ATOM	1016	CD1	LEU A 1		4.163	55.367	54.600		21.68
अर्थे कर वैकर	ATOM	1017	CD2				55.206	55.797		17.56
25	ATOM	1017	N	PHE A 1		4.222	55.008	53.380		13.86
	ATOM	1019	CA	PHE A 1		7.533	54.828	56.348		29.24
i de	ATOM	1019	CA	PHE A 1		8.129	53.527	56.323		33.44
	ATOM	1020	0			7.299	52.519	57.157		41.08
**	ATOM	1021	CB	PHE A 1		6.344	52.889	57.837		46.05
30	ATOM	1023	CG	PHE A 1		9.621	53.670	56.791		36.40
	ATOM	1023		PHE A 1		9.763	53.895	58.256		38.11
		1024		PHE A 1		9.601	52.821	59.053		37.18
	ATOM			PHE A 1		10.123	55.158	58.803		43.89
See at 1	MOTA	1026		PHE A 1		9.771	52.936	60.422		41.04
35	ATOM	1027 1028				10.289	55.258	60.174		47.72
hath J	ATOM		CZ	PHE A 1		10.131	54.143	60.986		44.34
	ATOM	1029 1030	N CA	SER A 1		7.612	51.221	57.002		33.47
	ATOM	1030	C	SER A 1		6.744	50.228	57.629		29.86
	ATOM	1031		SER A 1 SER A 1		7.499	49.221	58.504		31.53
40	ATOM	1032	O CB	SER A 1		8.724	49.146	58.531		33.16
40	ATOM	1033	OG			5.942	49.481	56.535		33.19
	ATOM	1034	N	SER A 1 GLN A 1		6.757	48.480	55.926		50.66
	ATOM	1035	CA	GLN A 1		6.703	48.466	59.294		24.61
	ATOM	1030	CA			7.283	47.422	60.134		22.55
45	ATOM	1037		GLN A 1		6.268	46.321	60.398		27.28
73	ATOM	1038	O CB	GLN A 1 GLN A 1		5.161	46.566	60.809		25.09
	ATOM	1040	CG	GLN A 1		7.711	48.041	61.464		23.29
	ATOM	1041	CD	GLN A 1		8.218	46.987	62.454		25.96
	ATOM	1041	OE1	GLN A 1		9.423	46.290	61.872		25.65
50	ATOM	1042	NE2			10.296	46.876	61.263		26.36
50	ATOM	1043	N			9.445	44.965	62.095		21.75
	ATOM	1044	CA	CYS A 1		6.435	45.124	59.820	1.00	29.60
	ATOM	1045	C	CYS A 1		5.291	44.220	59.755		32.30
	ATOM					5.442	43.006	60.662		39.58
55	ATOM	1047	O	CYS A 1		4.597	42.144	60.739		40.94
22		1048	CB	CYS A 1		5.098	43.794	58.320		35.40
	ATOM	1049	SG	CYS A 1		3.976	44.922	57.445		41.22
	ATOM	1050	N	GLN A 1		6.582	42.949	61.345		37.37
	ATOM	1051	CA	GLN A 1		6.715	41.982	62.417		35.71
60	ATOM	1052	C	GLN A 1		6.589	42.645	63.797		31.90
OU.	ATOM	1053	0	GLN A 1		6.878	43.803	63.981		30.54
	ATOM	1054	CB	GLN A 1		8.077	41.311	62.295		37.24
	ATOM	1055	CG	GLN A 1		8.076	39.878	62.847		29.70
	ATOM	1056	CD	GLN A 1		9.483	39.511	63.235		36.48
	ATOM	1057	OET	GLN A 1	.36	10.366	40.328	63.356	1.00	24.49

	MOTA MOTA MOTA MOTA	1058 1059 1060 1061	NE2 N CA C	GLN A ALA A ALA A ALA A	137 137	9.665 5.850 5.235 3.860	38.201 41.899 40.581 40.503	63.443 64.648 64.351	1.00 1.00	22.19 28.56 28.89
5	ATOM	1062	ō	ALA A		3.679	39.688	63.630 62.738		31.83 29.67
	ATOM	1063	CB	ALA A		5.091	39.742	65.625	1.00	28.91
	ATOM ATOM	1064 1065	N CA	ILE A		2.863 1.553	41.285 41.176	64.070 63.445		27.07
	ATOM	1066	C	ILE A		0.960	42.492	63.053		23.90 28.69
10	ATOM	1067	0	ILE A		-0.144	42.822	63.426		31.92
	ATOM ATOM	1068 1069	CB	ILE A		0.641	40.357	64.339		25.41
	ATOM	1009		ILE A		0.871 1.162	40.811 38.938	65.801		27.32
	ATOM	1071		ILE A		-0.275	40.615	64.191 66.826		16.34 20.22
15	ATOM	1072	N	HIS A	139	1.718	43.223	62.265		24.05
	ATOM	1073	CA	HIS A		1.322	44.511	61.824	1.00	24.05
	ATOM ATOM	1074 1075	С О	HIS A		0.982	44.579	60.351		34.40
E and	ATOM	1075	CB	HIS A		0.539 2.439	45.625 45.519	59.888 62.173		35.89
20	ATOM	1077	CG	HIS A		2.689	45.619	63.657		24.63 27.97
A.	ATOM	1078		HIS A		1.679	45.970	64.571		27.75
lad.	ATOM	1079		HIS A		3.835	45.437	64.356	1.00	28.42
15 Table 15 Table	ATOM ATOM	1080 1081		HIS A		2.222 3.517	45.983 45.668	65.770		26.19
25	ATOM	1082	N	CYS A		1.181	43.490	65.671 59.598		27.42 30.28
HA.	ATOM	1083	CA	CYS A	140	0.832	43.517	58.181		28.08
	ATOM	1084	C	CYS A		-0.671	43.765	58.011		28.98
₩ Le	ATOM ATOM	1085 1086	O	CYS A		-1.111	44.449	57.066		30.00
30	ATOM	1087	CB SG	CYS A		1.181 1.330	42.213 42.483	57.447 55.661		28.82
13	ATOM	1088	N	ARG A		-1.440	43.168	58.949		34.37 20.78
	ATOM	1089	CA	ARG A	141	-2.884	43.252	58.996		20.33
12 E	ATOM	1090	C	ARG A		-3.286	44.684	59.003	1.00	32.37
14 35	ATOM ATOM	1091 1092	O CB	ARG A		-4.355	45.032	58.510		35.81
, , ,	ATOM	1093	CG	ARG A		-3.557 -3.081	42.498 42.891	60.156 61.568		14.60 20.94
	ATOM	1094	CD	ARG A		-3.576	41.978	62.715		19.99
	ATOM	1095	NE	ARG A		-2.911	40.690	62.786		18.24
40	ATOM ATOM	1096 1097	CZ	ARG A		-3.140	39.707	63.648		18.77
, ,,	ATOM	1097		ARG A		-4.029 -2.415	39.739 38.640	64.634 63.508		20.76
	ATOM	1099	N	ALA A		-2.408	45.511	59.580		24.20 28.35
	ATOM	1100		ALA A		-2.668	46.940	59.657		27.60
45	ATOM ATOM	1101 1102	C	ALA A		-2.369	47.652	58.345		34.33
	ATOM	1102		ALA A		-2.620 -1.994	48.835 47.616	58.203 60.843		34.36
	ATOM	1104	N	ILE A		-1.824	46.922	57.382		27.67 32.39
	ATOM	1105	CA	ILE A		-1.537	47.499	56.099		30.38
50	ATOM	1106	C	ILE A		-2.520	46.994	55.067	1.00	37.79
. 50	ATOM ATOM	1107 1108	O CB	ILE A		-2.885 -0.142	47.709	54.152		42.65
	ATOM	1109		ILE A	143	0.827	47.228 48.062	55.613 56.414		32.06 31.71
	ATOM	1110	CG2	ILE A	143	-0.074	47.654	54.143		34.02
55	MOTA	1111		ILE A		2.258	47.774	55.988		42.10
23	ATOM ATOM	1112 1113		LEU A		-2.939	45.749	55.218		32.50
	ATOM	1114		LEU A		-3.873 -4.435	45.142 43.838	54.291 54.849		32.36
	MOTA	1115		LEU A		-3.959	43.278	55.852		40.36 33.27
۲0	ATOM	1116	CB	LEU A	144	-3.250	44.936	52.894		31.58
60	ATOM	1117		LEU A		-1.923	44.170	52.917	1.00	33.31
	"ATOM ATOM	1118 1119		LEU A		-2.147 -0.836	42.770	52.352		32.07
	ATOM	1120		PRO A		-0.836 -5.490	44.897 43.347	52.110 54.213	1.00	28.67
	MOTA	1121		PRO A		-6.080	42.129	54.715		37.86

	ATOM	1122	С	PRO A 145	-5.264	40.941	54.286	1.00 37.87
	ATOM	1123	0	PRO A 145	-4.819	40.831	53.144	1.00 37.07
	ATOM	1124	СВ	PRO A 145	-7.530	42.080	54.220	1.00 38.81
٠.	ATOM	1125	CG	PRO A 145	-7.778	43.393	53.492	1.00 38.81
. 5	ATOM	1126	CD	PRO A 145	-6.432	44.093	53.341	1.00 41.34
	ATOM	1127	N	CYS A 146	-5.041	40.056	55.233	1.00 36.89
	ATOM	1128	CA	CYS A 146	-4.250	38.882		
	ATOM	1129	c	CYS A 146	-4.358	37.859	54.958	1.00 35.60
	ATOM	1130	ŏ	CYS A 146	-5.067		56.069	1.00 33.04
10	ATOM	1131	СВ	CYS A 146		38.062	57.050	1.00 30.78
10	ATOM	1132	SG	CYS A 146	-2.761	39.287	54.813	1.00 36.08
	ATOM	1133	N	GLN A 147	-2.087	40.108	56.302	1.00 39.43
	ATOM	1134	CA	GLN A 147	-3.637	36.755	55.883	1.00 29.33
	ATOM	1134	CA	GLN A 147	-3.517	35.703	56.875	1.00 29.71
15					-2.254	36.131	57.628	1.00 38.75
13	MOTA	1136 1137	O	GLN A 147	-1.141	35.926	57.135	1.00 40.79
	ATOM		CB	GLN A 147	-3.322	34.352	56.206	1.00 28.99
HERE BEEN	ATOM	1138	CG	GLN A 147	-4.672	33.707	55.894	1.00 25.73
	ATOM	1139	CD	GLN A 147	-4.562	32.532	54.960	1.00 39.92
20	MOTA	1140	OE1	GLN A 147	-4.217	32.668	53.775	1.00 43.89
20	ATOM	1141		GLN A 147	-4.828	31.368	55.499	1.00 26.36
1=4 ₀	MOTA	1142	N	ASP A 148	-2.425	36.834	58.765	1.00 32.68
initia april America	ATOM	1143	CA	ASP A 148	-1.287	37.362	59.474	1.00 33.50
HARRY THE PARTY	ATOM	1144	С	ASP A 148	-0.629	36.377	60.371	1.00 33.13
明明のと	ATOM	1145	0	ASP A 148	-0.622	36.563	61.584	1.00 31.30
1 25	MOTA	1146	CB	ASP A 148	-1.633	38.642	60.253	1.00 37.78
ļ. 4 .	ATOM	1147	CG	ASP A 148	-0.535	39.666	60.332	1.00 45.10
#	MOTA	1148		ASP A 148	0.564	39.540	59.836	1.00 47.89
lah.	ATOM	1149		ASP A 148	-0.913	40.737	60.952	1.00 48.63
	MOTA	1150	N	THR A 149	-0.080	35.345	59.742	1.00 29.15
30	MOTA	1151	CA	THR A 149	0.584	34.251	60.422	1.00 28.25
1.00	ATOM	1152	С	THR A 149	1.805	33.831	59.625	1.00 34.92
	ATOM	1153	0	THR A 149	1.757	33.764	58.410	1.00 34.47
	ATOM	1154	CB	THR A 149	-0.403	33.087	60.674	1.00 24.79
35	ATOM	1155	OG1		0.241	32.059	61.352	1.00 37.15
35	ATOM	1156	CG2	THR A 149	-0.905	32.527	59.345	1.00 26.56
	ATOM	1157	N	PRO A 150	2.910	33.575	60.323	1.00 34.69
	MOTA	1158	CA ·	PRO A 150	4.142	33.217	59.659	1.00 31.06
	ATOM	1159	С	PRO A 150	4.087	31.813	59.131	1.00 36.66
40	ATOM	1160	0	PRO A 150	4.995	31.356	58.450	1.00 36.37
40	MOTA	1161	CB	PRO A 150	5.245	33.327	60.712	1.00 31.18
	ATOM	1162	CG	PRO A 150	4.570	33.471	62.077	1.00 36.95
	ATOM	1163	CD	PRO A 150	3.078	33.589	61.823	1.00 34.62
	MOTA	1164	N	SER A 151	2.992	31.150	59.452	1.00 31.62
	ATOM	1165	CA	SER A 151	2.778	29.791	59.029	1.00 27.35
45	MOTA	1166	C	SER A 151	2.357	29.738	57.564	1.00 32.97
	MOTA	1167	0	SER A 151	2.344	28.703	56.928	1.00 34.25
	ATOM	1168	CB	SER A 151	1.714	29.203	59.905	1.00 25.95
	ATOM	1169	OG	SER A 151	0.483	29.685	59.439	1.00 49.35
	ATOM	1170	N	VAL A 152	1.997	30.887	57.024	1.00 34.36
50	ATOM	1171	CA	VAL A 152	1.595	31.015	55.623	1.00 33.74
	ATOM	1172	С	VAL A 152	2.705	31.764	54.847	1.00 37.45
	ATOM	1173	0	VAL A 152	3.295	32.761	55.313	1.00 37.63
	ATOM	1174	CB	VAL A 152	0.203	31.697	55.427	1.00 32.61
	MOTA	1175	CG1	VAL A 152	-0.184	31.767	53.963	1.00 31.50
55	ATOM	1176	CG2	VAL A 152	-0.915	30.975	56.149	1.00 31.29
	ATOM	1177	N	LYS A 153	2.999	31.289	53.654	1.00 26.98
	ATOM	1178	CA	LYS A 153	4.002	31.927	52.866	1.00 25.81
	ATOM	1179	С	LYS A 153	3.469	32.141	51.473	1.00 23.81
	ATOM	1180	0	LYS A 153	2.826	31.251	50.936	1.00 33.94
60	ATOM	1181	СВ	LYS A 153	5.252	31.091	52.841	
	ATOM	1182	CG	LYS A 153	6.383	31.760	53.583	1.00 24.70
	ATOM	1183	CD	LYS A 153	7.641	30.893	53.563	1.00 34.68
	ATOM	1184	CE	LYS A 153	8.121	30.506		1.00 39.37
	ATOM	1185	NZ	LYS A 153	9.556	30.152	55.015	1.00 29.09
					2.330	20.125	55.112	1.00 26.03

	ATOM	1186	N	LEU A	154	3.732	33.321	50.896	1.00 32.13
	ATOM	1187	CA	LEU A		3.285	33.639		
								49.544	1.00 30.67
	ATOM	1188	С	LEU A		4.279	34.475	48.789	1.00 40.67
	ATOM	1189	0	LEU A	154	5.264	35.000	49.344	1.00 42.56
5	ATOM	1190	СВ	LEU A					
J.						1.966	34.432	49.515	1.00 30.10
	ATOM	1191	CG	LEU A	154	2.084	35.793	50.207	1.00 35.20
	MOTA	1192	CD1	LEU A	154	0.989	36.716	49.690	1.00 37.21
	ATOM	1193		LEU A		1.934	35.608	51.715	1.00 33.07
	ATOM	1194	N	THR A	155	3.963	34.610	47.499	1.00 37.82
10	ATOM	1195	CA	THR A		4.728	35.449	46.596	
10									1.00 38.44
	ATOM	1196	С	THR A	155	3.934	36.730	46.389	1.00 41.52
	ATOM	1197	0	THR A	155	2.738	36.775	46.674	1.00 43.95
	ATOM	1198	CB	THR A		5.041	34.814		
								45.230	1.00 36.99
1.5	ATOM	1199	OGI	THR A	155	3.886	34.281	44.584	1.00 32.59
15	ATOM	1200	CG2	THR A	155	6.133	33.790	45.404	1.00 18.24
	ATOM	1201	N	TYR A					
						4.563	37.768	45.892	1.00 33.87
	ATOM	1202	CA	TYR A	156	3.835	39.003	45.683	1.00 32.49
	ATOM	1203	С	TYR A	156	4.509	39.922	44.717	
									1.00 37.91
20	ATOM	1204	0	TYR A		5.725	39.940	44.562	1.00 39.04
20	MOTA	1205	CB	TYR A	156	3.534	39.795	46.983	1.00 31.16
	ATOM	1206	CG	TYR A		4.642	40.731		
								47.471	1.00 28.94
	ATOM	1207	CD1			4.817	42.021	46.969	1.00 30.33
	ATOM	1208	CD2	TYR A	156	5.525	40.303	48.465	1.00 30.43
	MOTA	1209	CE1	TYR A					
25						5.829	42.853	47.459	1.00 36.89
25	ATOM	1210	CE2	TYR A	156	6.553	41.104	48.960	1.00 31.47
	ATOM	1211	CZ	TYR A	156	6.690	42.396	48.462	1.00 43.34
	ATOM	1212	ОН	TYR A					
						7.701	43.180	48.956	1.00 36.86
	ATOM	1213	N	THR A	157	3.657	40.689	44.101	1.00 36.75
	ATOM	1214	CA	THR A	157	4.036	41.691	43.171	1.00 38.49
30	ATOM	1215	С	THR A					
50						3.346	42.942	43.611	1.00 42.61
	ATOM	1216	0	THR A	157	2.228	42.913	44.143	1.00 38.45
	ATOM	1217	CB	THR A	157	3.631	41.316	41.751	1.00 39.73
	ATOM	1218		THR A					
						2.380	40.655	41.803	1.00 55.71
	ATOM	1219	CG2	THR A	157	4.680	40.370	41.212	1.00 26.71
35	ATOM	1220	N	ALA A	158	4.037	44.025	43.404	1.00 41.36
	ATOM	1221	CA						
				ALA A		3.488	45.273	43.789	1.00 41.08
	ATOM	1222	C	ALA A	158	3.869	46.401	42.839	1.00 50.77
	ATOM	1223	0	ALA A	158	4.919	46.390	42.179	1.00 53.47
	ATOM	1224	CB	ALA A			45.570		
40						3.910		45.212	1.00 39.87
40	ATOM	1225	N	GLU A	159	2.974	47.376	42.788	1.00 43.90
	ATOM	1226	CA	GLU A	159	3.107	48.604	42.023	1.00 42.27
	ATOM	1227	С	GLU A	15Q	2.451	49.705		
								42.843	1.00 42.17
	ATOM	1228	0	GLU A	128	1.257	49.630	43.227	1.00 41.00
	ATOM	1229	CB	GLU A	159	2.641	48.521	40.571	1.00 43.72
45	ATOM	1230	CG	GLU A	159		47.197		
								40.255	1.00 62.90
	MOTA	1231	CD	GLU A		1.502	47.156	38.835	1.00 91.28
	ATOM	1232	OE1	GLU A	159	2.202	46.696	37.955	1.00 77.84
	ATOM	1233		GLU A		0.322			
							47.707	38.644	1.00100.00
50	ATOM	1234	N	VAL A	160	3.263	50.686	43.197	1.00 34.67
- 50	ATOM	1235	CA	VAL A	160	2.738	51.717	44.044	1.00 36.57
	ATOM	1236	С	VAL A		3.024	53.091		
								43.533	1.00 43.02
	ATOM	1237	0	VAL A	100	4.121	53.380	43.050	1.00 42.71
	MOTA	1238	CB	VAL A	160	3.180	51.530	45.500	1.00 40.73
	ATOM	1239		VAL A					
55						3.988	50.239	45.644	1.00 38.56
55	MOTA	1240		VAL A		4.006	52.728	45.963	1.00 40.46
	ATOM	1241	N	SER A	161	2.002	53.922	43.653	1.00 41.79
	ATOM	1242	CA	SER A		2.076			
							55.292	43.185	1.00 42.07
	ATOM	1243	С	SER A	101	2.532	56.204	44.270	1.00 44.28
1 -	ATOM	1244	0	SER A	161	2.047	56.121	45.403	1.00 43.60
60	ATOM	1245	СВ	SER A		0.751			
-							55.801	42.635	1.00 43.32
	ATOM	1246	OG	SER A		0.971	56.850	41.726	1.00 49.40
	MOTA	1247	N	VAL A	162	3.447	57.080	43.896	1.00 36.49
	ATOM	1248	CA	VAL A		3.979	58.019	44.838	
									1.00 34.99
	ATOM	1249	C	VAL A	1.07	4.273	59.319	44.148	1.00 42.57

	ATOM	1250	^	3.73 T	7	100		4 400				
			0	VAL				4.470	59.354	42.932	1.00 4	
	MOTA	1251	CB			162		5.300	57.498	45.402	1.00 3	5.97
	ATOM	1252	CG1	VAL	Α	162		5.084	56.219	46.188	1.00 3	
	MOTA	1253		VAL				6.222	57.194	44.239	1.00 3	E 40
5	ATOM	1254	N			163						
J. J.								4.332	60.377	44.942	1.00 3	
	ATOM	1255	CA			163		4.664	61.662	44.400	1.00 3	1.07
	MOTA	1256	С	PRO	Α	163		5.966	61.496	43.652	1.00 3	9 67
	ATOM	1257	0			163		6.919	60.892	44.142		
	ATOM	1258	СВ			163					1.00 4	
10								4.780	62.562	45.618	1.00 3	1.62
10	MOTA	1259	CG			163		3.946	61.893	46.714	1.00 3	3.93
	ATOM	1260	CD	PRC	Α	163		3.652	60.480	46.259	1.00 2	
	ATOM	1261	N	LYS	А	164		5.962	61.978	42.436	1.00 3	
	ATOM	1262	CA	LYS				7.086				
									61.860	41.539	1.00 3	
1.5	ATOM	1263	С	LYS				8.451	62.222	42.088	1.00 4	2.75
15	ATOM	1264	0	LYS	Α	164		9.453	61.708	41.593	1.00 4	4.47
	MOTA	1265	CB	LYS	Α	164		6.828	62.479	40.177	1.00 4	
	ATOM	1266	CG	LYS								
								6.004	63.758	40.257	1.00 7	8.05
	MOTA	1267	CD	LYS				6.651	64.918	39.497	1.0010	0.00
, iffo.	MOTA	1268	CE	LYS	A	164		6.016	66.289	39.772	1.0010	0.00
20	ATOM	1269	NZ	LYS	Α	164		6.679	67.075	40.835	1.0010	
4320	ATOM	1270	N	GLU								
1.4.	ATOM	1271						8.519	63.097	43.082	1.00 3	
			CA	GLU				9.814	63.489	43.665	1.00 3	9.56
ing into	ATOM	1272	С	GLU	Α	165	•	10.333	62.462	44.677	1.00 4	6.39
2 9R4,	ATOM	1273	0	GLU	Α	165		11.531	62.318	44.927	1.00 4	
25	ATOM	1274	CB	GLU				9.797	64.902			
	ATOM	1275								44.297	1.00 4	
} =			CG	GLU				8.602	65.156	45.257	1.00 5	8.16
110	ATOM	1276	CD	GLU				7.214	64.970	44.664	1.00 8	8.01
IN	ATOM	1277	OE1	GLU	Α	165		6.994	64.757	43.475	1.00 7	
- #-	 ATOM	1278	OE2	GLU				6.266	65.050			
130	ATOM	1279	N	LEU						45.575	1.00 7	
								9.398	61.733	45.265	1.00 4	
n.	ATOM	1280	CA	LEU				9.696	60.733	46.254	1.00 3	6.56
C.	ATOM	1281	С	LEU	Α	166		9.934	59.377	45.640	1.00 4	
	ATOM	1282	0	LEU	А	166		9.366	59.080	44.581	1.00 5	
See Mile	ATOM	1283	СВ	LEU								
35								8.525	60.630	47.250	1.00 3	
33	MOTA	1284	CG	LEU	А	100		8.315	61.912	48.057	1.00 2	9.18
	ATOM	1285		LEU				7.363	61.590	49,189	1.00 2	5.96
	ATOM	1286	CD2	LEU	Α	166		9.635	62.467	48.622	1.00 2	
	ATOM	1287	N	VAL				10.769	58.564	46.328		
	ATOM	1288	CA	VAL							1.00 3	
40								11.077	57.218	45.908	1.00 3	0.00
40	ATOM	1289	С	VAL	А	167		10.332	56.229	46.771	1.00 3	8.80
	MOTA	1290	0	VAL	А	167		9.902	56.532	47.879	1.00 4	n 91
	ATOM	1291	CB	VAL	Α	167		12.549	56.860	46.048	1.00 3	
	ATOM	1292	CG1					12.854	55.542			
										45.329	1.00 2	8.20
15	ATOM	1293		VAL				13.456	57.964	45.565	1.00 3	1.06
45	ATOM	1294	N	ALA				10.217	55.019	46.257	1.00 3	6.46
	ATOM	1295	CA	ALA	A	168		9.584	53.935	46.979	1.00 3	
	ATOM	1296	С	ALA				10.418	52.662			
	ATOM	1297	Ö	ALA						46.836	1.00 4	
								10.889	52.343	45.733	1.00 4	4.74
50	ATOM	1298	CB	ALA				8.149	53.700	46.550	1.00 3	4.20
50	ATOM	1299	N	LEU	Α	169		10.603	51.960	47.975	1.00 3	
	ATOM	1300	CA	LEU	Α	169		11.323	50.696	48.069	1.00 2	
	MOTA	1301	С	LEU				10.491				
									49.635	48.797	1.00 3	3.87
	MOTA	1302	0	LEU				9.604	49.918	49.613	1.00 3	1.21
	ATOM	1303	CB	LEU	A	169		12.721	50.835	48.656	1.00 2	
55	ATOM	1304	CG	LEU	Α	169		13.593	51.810	47.891	1.00 3	
	ATOM	1305		LEU				14.953				
	ATOM	1306							51.819	48.558	1.00 3	
				LEU				13.765	51.394	46.432	1.00 3	
	MOTA	1307	N	MET				10.758	48.381	48.479	1.00 3	
	ATOM	1308	CA	MET	Α	170		10.012	47.291	49.069	1.00 3	
60	MOTA	1309	С	MET				10.874	46.083			
	ATOM	1310	ō	MET						49.287	1.00 3	
								11.995	45.973	48.775	1.00 3	
	ATOM	1311	CB	MET	Α	T 10		8.842	46.882	48.154	1.00 3	1.95
	ATOM	1312	CG	MET				7.751	47.934	48.116	1.00 3	
	MOTA	1313	SD	MET	Α	170		6.105	47.253	47.815	1.00 3	
											# 1 0 0 J	

		MOTA	1314	CE	MET :	A	170	5.820	46.349	49.363	1.00 32.25
		ATOM	1315	N	SER			10.332	45.165	50.057	1.00 28.20
		ATOM	1316	CA	SER			11.064	43.953	50.297	1.00 28.47
		ATOM	1317	С	SER			10.929	43.054	49.049	1.00 32.01
	5	ATOM	1318	Ō	SER			10.396	41.958	49.089	1.00 30.93
	-	ATOM	1319	СВ	SER .			10.662	43.265	51.606	1.00 30.93
		ATOM	1320	OG	SER .			9.297	42.920	51.581	
		ATOM	1321	N	ALA .			11.401	42.920		1.00 32.90
		ATOM	1322	CA						47.912	1.00 28.84
	10				ALA .			11.286	42.773	46.691	1.00 29.48
	10	ATOM	1323	С	ALA .			12.241	43.258	45.644	1.00 37.63
		MOTA	1324	0	ALA.			13.060	44.147	45.881	1.00 35.07
		ATOM	1325	CB	ALA .		_	9.884	42.969	46.120	1.00 29.48
		MOTA	1326	N	ILE .			12.104	42.686	44.452	1.00 39.49
		ATOM	1327	CA	ILE .			12.966	43.120	43.382	1.00 38.64
,	15	MOTA	1328	С	ILE .	A	173	12.418	44.343	42.648	1.00 44.83
		ATOM	1329	0	ILE .	A	173	11.269	44.394	42.193	1.00 40.97
		MOTA	1330	CB	ILE .	Α	173	13.549	42.027	42.479	1.00 38.79
		ATOM	1331	CG1	ILE .	A	173	14.258	40.970	43.302	1.00 37.40
Cis		ATOM	1332	CG2	ILE .	Α	173	14.606	42.621	41.570	1.00 38.88
	20	ATOM	1333		ILE .			15.770	41.069	43.193	1.00 25.93
714 mg/s		ATOM	1334	N	ARG .			13.286	45.345	42.584	1.00 43.21
1-4-		ATOM	1335	CA	ARG			12.997	46.567	41.917	1.00 42.34
140 ±10 142 ±10 143 ±10		ATOM	1336	C	ARG .			12.630	46.173	40.516	1.00 47.54
3 5FA 14 5 5FA		ATOM	1337	Õ	ARG .			13.478	45.667	39.770	1.00 47.34
UT :	25	ATOM	1338	СВ	ARG .			14.254	47.422		
3=50		ATOM	1339	CG	ARG .					41.937	1.00 42.47
								14.231	48.450	43.075	1.00 53.40
189		ATOM	1340	CD	ARG .			15.617	48.917	43.515	1.00 33.80
4		MOTA	1341	NE	ARG .			16.036	50.083	42.756	1.00 53.32
na.	30	ATOM	1342	CZ	ARG .			17.221	50.208	42.181	1.00 97.11
n.	30	ATOM	1343		ARG .			18.132	49.243	42.266	1.00100.00
24 mg		MOTA	1344		ARG .			17.503	51.321	41.489	1.00100.00
en str.		MOTA	1345	N	ASP .			11.356	46.356	40.195	1.00 51.12
		MOTA	1346	CA	ASP .			10.858	45.981	38.882	1.00 53.89
Jak.	25	MOTA	1347	С	ASP .			10.778	47.128	37.885	1.00 58.32
*	35	MOTA	1348	0	ASP .			10.455	46.901	36.727	1.00 56.00
		ATOM	1349	CB	ASP .			9.533	45.186	38.948	1.00 57.16
		ATOM	1350	CG	ASP .			9.196	44.446	37.675	1.00 81.25
		ATOM	1351		ASP .			10.034	44.118	36.851	1.00 83.53
	4.0	ATOM	1352	OD2	ASP .	Α	175	7.910	44.176	37.558	1.00 92.45
•	40	MOTA	1353	N	GLY .	Α	176	11.062	48.356	38.331	1.00 58.24
		ATOM	1354	CA	GLY .	Α	176	11.021	49.498	37.438	1.00 57.71
		MOTA	1355	С	GLY .	Α	176	9.969	50.546	37.773	1.00 58.98
		MOTA	1356	0	GLY .	Α	176	9.090	50.371	38.620	1.00 52.04
		MOTA	1357	N	GLU .	Α	177	10.110	51.649	37.050	1.00 63.72
	45	MOTA	1358	CA	GLU .	Α	177	9.267	52.812	37.172	1.00 67.79
		ATOM	1359	С	GLU .	Α	177	8.874	53.388	35.817	1.00 86.22
		ATOM	1360	0	GLU .			9.614	53.364	34.830	1.00 91.14
		MOTA	1361	CB	GLU .	Α	177	9.986	53.902	38.006	1.00 68.25
		MOTA	1362	CG	GLU .			11.432	54.145	37.519	1.00 71.58
	50	ATOM	1363	CD	GLU .			12.183	55.088	38.404	1.00 85.08
		MOTA	1364		GLU .	A	177	13.045	54.733	39.198	1.00100.00
		ATOM	1365	OE2	GLU			11.765	56.316	38.264	1.00 56.71
		ATOM	1366	N	THR			7.671	53.924	35.835	1.00 84.76
		ATOM	1367	CA	THR			6.684	54.686	35.033	
	55	ATOM	1368	C	THR					35.855	1.00 84.81
	<i>J J</i>	ATOM	1369		THR			6.024	55.810		1.00 90.37
				O				5.664	55.655	36.996	1.00 91.10
		ATOM	1370	CB	THR .			5.618	53.713	34.561	1.00 89.82
		ATOM	1371		THR			5.283	52.830	35.636	1.00 80.25
	6 0	ATOM	1372		THR .			6.161	52.898	33.396	1.00 93.46
	60	MOTA	1373	N	PRO			5.921	56.984	35.217	1.00 87.05
		ATOM	1374	CA	PRO			5.365	58.187	35.845	1.00 86.61
		ATOM	1375	С	PRO			3.857	58.419	35.531	1.00 89.04
		MOTA	1376	0	PRO			3.444	59.516	35.140	1.00 91.15
		MOTA	1377	CB	PRO	A	179	6.176	59.345	35.301	1.00 88.63

	MOTA	1378	CG	PRO A	179	6.657	58.947	33.895	1.00 92.62
	ATOM	1379	CD	PRO A	179	6.426	57.345	33.902	1.00 87.63
	ATOM	1380	N	ASP A	180	3.020	57.347	35.694	1.00 82.31
	ATOM	1381	CA	ASP A		1.616	57.568	35.310	1.00 81.19
5	MOTA	1382	С	ASP A		0.629	56.743	36.166	1.00 90.72
	ATOM	1383	0	ASP A		0.533	55.519	36.072	1.00 91.13
	ATOM	1384	CB	ASP A		1.458	57.196	33.827	1.00 82.12
	ATOM	1385	CG	ASP A		0.087	57.651	33.327	1.00 95.94
10	MOTA	1386		ASP A		-0.155	58.858	33.337	1.00100.00
10	MOTA	1387		ASP A		-0.714	56.801	32.946	1.00 94.36
	ATOM	1388	N	PRO A		-0.060	57.456	37.086	1.00 92.45
	MOTA	1389	CA	PRO A		-1.212	56.934	37.795	1.00 92.02
	ATOM	1390	C	PRO A		-2.519	57.566	37.284	1.00100.00
15	ATOM	1391	0	PRO A		-2.605	58.114	36.192	1.00100.00
15	ATOM	1392	CB	PRO A		-1.014	57.340	39.210	1.00 92.48
	ATOM	1393	CG CD	PRO A		-0.362	58.734	39.152	1.00 98.39
	ATOM	1394 1395	N	PRO A		0.268	58.736	37.663	1.00 94.17
	ATOM ATOM	1396	CA	GLU A		-3.567 -4.822	57.456 58.161	38.141	1.00100.00
20	ATOM	1397	C	GLU A		-5.359	58.856	37.876 39.154	1.00 98.21 1.00100.00
43	ATOM	1398	0	GLU A		-6.404	59.497	39.167	1.00100.00
jak,	ATOM	1399	CB	GLU A		-5.854	57.142	37.356	1.00 99.44
25 m/ 1 m/	ATOM	1400	CG	GLU A		-5.880	57.077	35.816	
\$200 #\$ 000	ATOM	1401	CD	GLU A		-7.013	57.938	35.300	1.00100.00
25	ATOM	1402	OE1	GLU A		-7.817	58.385	36.105	1.00100.00
	ATOM	1403	OE2	GLU A		-7.084	58.153	34.091	1.00100.00
ješ.	ATOM	1404	N	ASP A		-4.607	58.672	40.265	1.00 98.63
#	ATOM	1405	CA	ASP A		-5.021	59.257	41.552	1.00 97.49
\$= £0	ATOM	1406	C	ASP A		-4.126	60.472	41.932	1.00100.00
1.30	ATOM	1407	ō	ASP A		-3.464	61.061	41.079	1.00100.00
	ATOM	1408	СВ	ASP A		-4.946	58.144	42.619	1.00 98.36
	ATOM	1409	CG	ASP A		-3.612	57.409	42.547	1.00100.00
THE REP.	MOTA	1410	OD1	ASP A		-3.471	56.556	41.668	1.00100.00
12.0	ATOM	1411		ASP A		-2.741	57.688	43.364	1.00100.00
35	MOTA	1412	N	PRO A		-4.187	60.906	43.237	1.00 97.96
	MOTA	1413	CA	PRO A	184	-3.311	61.985	43.738	1.00 97.92
	ATOM	1414	С	PRO A	184	-1.865	61.528	44.071	1.00 97.89
	ATOM	1415	0	PRO A	184	-1.348	61.748	45.159	1.00100.00
4.0	MOTA	1416	CB	PRO A	184	-3.973	62.561	44.992	1.00 98.86
40	MOTA	1417	CG	PRO A		-5.262	61.777	45.284	1.00100.00
	ATOM	1418	CD	PRO A		-5.122	60.532	44.284	1.00 97.20
	ATOM	1419	N	SER A		-1.249	60.840	43.071	1.00 82.40
	ATOM	1420	CA	SER A		0.196	60.496	43.086	1.00 75.26
45	ATOM	1421	C	SER A		0.748	60.563	41.623	1.00 71.84
43	ATOM	1422	0	SER A		-0.006	60.525	40.670	1.00 77.97
	ATOM	1423	CB	SER A		0.337	59.068	43.636	1.00 73.41
	ATOM ATOM	1424 1425	OG N	SER A		0.672	59.109	45.027	1.00 63.60
	ATOM	1425	N CA	ARG A		2.107	60.704	41.461	1.00 57.89
50	ATOM	1427	CA	ARG A		2.650	60.971	40.088	1.00 56.00
50	ATOM	1428	o	ARG A		3.725 4.473	59.943 60.157	39.633 38.688	1.00 59.64
	ATOM	1429	СВ	ARG A		3.258	62.393	40.064	1.00 60.30 1.00 63.74
	ATOM	1430	CG	ARG A		2.339	63.457	40.677	1.00 80.44
	ATOM	1431	CD	ARG A		1.188	63.874	39.736	1.00 71.31
55	ATOM	1432	NE	ARG A		1.316	63.215	38.436	1.00 71.51
-	ATOM	1433	CZ	ARG A		0.185	62.862	37.784	1.00 95.30
	ATOM	1434		ARG A		-0.999	63.109	38.312	1.00 56.25
	ATOM	1435		ARG A		0.276	62.232	36.603	1.00 89.98
	MOTA	1436	N	LYS A		3.892	58.778	40.265	1.00 54.50
60	ATOM	1437	CA	LYS A		4.891	57.805	39.851	1.00 51.93
	ATOM	1438	С	LYS A		4.506	56.436	40.276	1.00 52.96
	MOTA	1439	0	LYS A		3.971	56.236	41.368	1.00 53.58
	MOTA	1440	CB	LYS A		6.247	58.047	40.470	1.00 53.78
	ATOM	1441	CG	LYS A		7.427	57.714	39.574	1.00 43.05

		AT	OM	1442	CD	LYS	Α	187		8.517	5	8.761	30	.762	1 00	53.36
		AT		1443	CE	LYS				9.870		8.468		.146		39.68
•		AT		1444	NZ	LYS				10.795		9.601		341		40.19
		AT		1445	N	ILE				4.819		5.502		.403		46.36
	5	AT		1446	CA	ILE										
	7									4.565		4.128		700		43.57
		AT		1447	C	ILE				5.824		3.311		851		42,64
		AT		1448	0	ILE			•	6.647		3.189		3.937		41.55
		AT		1449	CB	ILE				3.579		3.425	38	3.826		45.64
		AT	OM	1450		ILE				2.193	5	4.021	39	0.047	1.00	45.82
	10	AT	OM	1451	CG2	ILE	Α	188		3.590	5	1.969	39	.273	1.00	43.43
		AT	OM	1452	CD1	ILE	Α	188		1.448	5	3.505	40	.276		62.08
		AT	OM	1453	N	TYR	Α	189		5.950		2.757		.042		35.58
		AT		1454	CA	TYR				7.079		1.933		.356		37.57
		AT		1455	C	TYR				6.652		0.465		.359		44.89
	15	AT		1456	Ö	TYR				5.656		0.092		.999		44.33
	10	AT		1457	CB	TYR				7.752		2.392				
			OM	1458	CG	TYR								2.661		37.85
ar su										8.692		3.563		2.456		34.49
			OM	1459		TYR				9.968		3.375		.930		35.93
	00		MO	1460	CD2					8.310		4.859		2.813	1.00	32.44
T. T.	20		OM	1461		TYR				10.843		4.449	41	.753		36.88
34 #0		AT	OM	1462	CE2	TYR	A	189		9.170	5	5.945	42	2.647	1.00	31.63
1-4		TA	OM	1463	CZ	TYR	Α	189		10.441	. 5	5.734	42	2.113	1.00	44.54
1984 1984 1984		AT	MO	1464	OH	TYR	Α	189		11.296	5	6.788	41	.929		57.77
15 THE			MO	1465	N	LYS	Α	190		7.413		9.651		.608		42.91
	25		OM	1466	CA	LYS				7.173		8.210		.420		42.22
-A			'OM	1467	С	LYS				8.152		7.262		1.143		40.73
in the			MO	1468	ō	LYS				9.398		7.400		1.093		35.69
#			'OM	1469	СВ	LYS				7.007		7.839				
]+#x				1470	CG									3.944		45.87
	30		MO			LYS				5.735		8.403		3.306		71.08
6 . Mar.	30		OM	1471	CD	LYS				5.758		8.384		5.779		84.62
			MO	1472	CE	LYS				4.386		8.157		5.147		100.00
			'OM	1473	NZ	LYS				4.299		6.930		.329		100.00
			'OM	1474	N	PHE				7.539	4	6.264	4]	1.812	1.00	35.01
3 5		AT	'OM	1475	CA	PHE	Α	191		8.276	4	5.304	42	2.592	1.00	31.57
#	35	AT	'OM	1476	С	PHE	Α	191		7.792	2 4	3.871	42	2.465	1.00	30.89
		AT	'OM	1477	0	PHE	Α	191		6.603	3 4	3.584	42	2.377		25.06
		AT	'OM	1478	CB	PHE	Α	191		8.217	4	5.734	44	1.080		32.11
		AT	'OM	1479	CG	PHE	Α	191		8.570		7.190		1.372		29.24
		AT	MO.	1480	CD1	PHE	Α	191		9.895		7.593		1.539		31.81
	40	AT	'OM	1481		PHE				7.565		8.147		1.508		30.17
			MO'	1482		PHE				10.230		8.925		1.805		34.10
			'OM	1483		PHE				7.866		9.483		1.776		33.69
			'OM	1484	CZ	PHE				9.201						
			OM	1485	N N	ILE						9.860		1.928		33.32
	45				-					8.764		2.961		2.505		35.75
	43		'OM	1486	CA	ILE				8.525		1.520		2.415		37.02
			MO'	1487	C	ILE				9.255		0.653		3.469		33.05
			'OM	1488	0	ILE				10.489		0.672		3.593		30.73
			MO	1489	CB	ILE				8.850		0.970		L.025		42.45
			MO	1490		ILE				8.289	4	1.914	39	9.981	1.00	46.39
	50	ΙA	MO	1491	CG2	ILE	A	192		8.251	. 3	9.567	4 (0.859	1.00	44.02
		ΑΊ	MO.	1492	CD1	ILE	A	192		7.609	4	1.231	38	3.798	1.00	69.61
		ΑI	MO	1493	N	GLN	Α	193		8.459	3	9.864	44	1.195		27.51
		ΙA	MO	1494	CA	GLN	Α	193		8.954		8.908		5.177		32.05
		AT	MO.	1495	С	GLN	Α	193		8.626		7.488		1.757		44.32
	55	- AT	MO	1496	0	GLN				7.583		6.926		.120		43.11
			MO	1497	СВ			193		8.502		9.100		5.638		33.44
			OM	1498	CG			193		9.285		8.203		7.632		22.34
			OM	1499	CD			193		10.824						
			OM	1500		GLN						8.337		7.636		48.52
	60									11.557		7.537		7.016		45.24
	UŲ		MO	1501		GLN				11.326		9.330		3.373		24.82
			MO	1502	N	LYS				9.543		6.908		3.993		46.91
			MO	1503	CA	LYS				9.384		5.540		3.529		47.56
			MO	1504	C	LYS				9.456		4.524		1.666		49.56
		ra.	MOT	1505	0	LYS	Α	194		8.777	7 3	3.520	44	1.598	1.00	50.85

	ATOM	1506	СВ	LYS A 194	10.385	35.159	42.439	1.00 48.11
	ATOM	1507	CG	LYS A 194	9.884	35.443	41.031	1.00 55.70
	ATOM	1508	CD	LYS A 194	10.895	36.200	40.179	1.00 67.67
	ATOM	1509	CE	LYS A 194	10.614	36.122	38.682	1.00 81.92
5	ATOM	1510	NZ	LYS A 194	11.284	37.185	37.910	1.00 88.34
	ATOM	1511	N	VAL A 195	10.308	34.753	45.689	1.00 39.55
	ATOM	1512	CA	VAL A 195	10.422	33.780	46.764	1.00 33.56
	MOTA	1513	С	VAL A 195	9.261	33.862	47.698	1.00 35.67
	MOTA	1514	0	VAL A 195	8.804	34.945	48.034	1.00 38.69
10	ATOM	1515	CB	VAL A 195	11.716	33.844	47.560	1.00 32.62
	MOTA	1516	CG1	VAL A 195	11.849	32.539	48.310	1.00 32.40
	ATOM	1517	CG2	VAL A 195	12.933	34.029	46.667	1.00 30.55
	ATOM -	1518	N	PRO A 196	8.770	32.717	48.126	1.00 27.75
	ATOM	1519	CA	PRO A 196		32.757	49.038	1.00 26.18
15	ATOM	1520	С	PRO A 196		33.236	50.410	1.00 35.86
	ATOM	1521	0	PRO A 196		32.809	50.899	1.00 35.43
	ATOM	1522	CB	PRO A 196		31.359	49.044	1.00 26.04
	MOTA	1523	CG	PRO A 196	7.856	30.472	48.113	1.00 27.79
.dec 20.	MOTA	1524	CD	PRO A 196		31.352	47.546	1.00 25.40
20	ATOM	1525	N	ILE A 197		34.171	51.009	1.00 29.92
43	ATOM	1526	CA	ILE A 197		34.697	52.284	1.00 26.98
	ATOM	1527	С	ILE A 197		34.809	53.128	1.00 34.88
j. L	ATOM	1528	0	ILE A 197		34.788	52.606	1.00 29.68
· P	ATOM	1529	СВ	ILE A 197		36.100	52.094	1.00 27.90
25	ATOM	1530		ILE A 197		36.867	51.254	1.00 27.78
B 1885	ATOM	1531	CG2			36.091	51.337	1.00 28.12
	ATOM	1532		ILE A 197		38.378	51.438	1.00 19.03
hot.	MOTA	1533	N	PRO A 198		34.936	54.447	1.00 36.02
52	ATOM	1534	CA	PRO A 198		35.110	55.410	1.00 31.31
30	MOTA	1535	С	PRO A 198		36.583	55.308	1.00 28.27
25T 12	ATOM	1536	0	PRO A 198		37.391	55.115	1.00 22.70
	ATOM	1537	CB	PRO A 198		34.849	56.794	1.00 31.17
	ATOM	1538	CG	PRO A 198		34.768	56.615	1.00 34.94
\$= #F	ATOM	1539	CD	PRO A 198		34.706	55.122	1.00 32.99
35	ATOM	1540	N	CYS A 199	4.011	36.939	55.405	1.00 27.60
la la	MOTA	1541	CA	CYS A 199	3.555	38.360	55.289	1.00 27.66
	ATOM	1542	С	CYS A 199		39.390	56.187	1.00 30.13
	ATOM	1543	0	CYS A 199		40.596	55.895	1.00 29.50
	ATOM	1544	CB	CYS A 199	2.025	38.534	55.242	1.00 27.18
40	ATOM	1545	SG	CYS A 199		38.279	56.841	1.00 30.85
	ATOM	1546	N	TYR A 200		38.903	57.270	1.00 26.15
	ATOM	1547	CA	TYR A 200	5.538	39.798	58.123	1.00 28.28
	ATOM	1548	С	TYR A 200	6.760	40.395	57.483	1.00 32.29
-	ATOM	1549	0	TYR A 200	7.359	41.286	58.036	1.00 31.56
45	ATOM	1550	CB	TYR A 200	5.844	39.215	59.489	1.00 30.59
	MOTA	1551	CG	TYR A 200	6.989	38.272	59.568	1.00 28.28
	MOTA	1552	CD1	TYR A 200	8.288	38.733	59.689	1.00 29.48
	ATOM	1553	CD2	TYR A 200	6.756	36.903	59.475	1.00 27.55
	ATOM	1554		TYR A 200		37.862	59.825	1.00 21.42
50	ATOM	1555		TYR A 200	7.838	36.015	59.595	1.00 27.41
	ATOM	1556	CZ	TYR A 200		36.488	59.737	1.00 25.11
	ATOM	1557	OH	TYR A 200		35.614	59.880	1.00 27.62
	ATOM	1558	N	LEU A 201		39.897	56.313	1.00 31.66
~ ~	ATOM	1559	CA	LEU A 201		40.378	55.579	1.00 29.49
55	MOTA	1560	С	LEU A 201		41.343	54.484	1.00 33.65
	MOTA	1561	0	LEU A 201		41.737	53.686	1.00 35.31
	ATOM	1562	CB	LEU A 201		39.275	55.035	1.00 27.04
	MOTA	1563	CG	LEU A 201		38.271	56.071	1.00 27.42
CA	ATOM	1564		LEU A 201		37.030	55.390	1.00 23.71
60	ATOM	1565		LEU A 201		38.913	56.957	1.00 30.55
	MOTA	1566	N	ILE A 202		41.710	54.438	1.00 28.66
	ATOM	1567	CA	ILE A 202		42.674	53.433	1.00 29.57
	ATOM	1568	C	ILE A 202		44.074	53.951	1.00 40.28
	ATOM	1569	0 ,	ILE A 202	6.192	44.493	55.027	1.00 40.75

	MOTA	1570	CB	ILE A	202	4.733	42.651	53.182	1.00 31.18
	MOTA	1571	CG1	ILE A		4.250	41.429	52.405	1.00 28.21
	ATOM	1572		ILE A		4.259	43.962	52.521	1.00 29.23
	ATOM	1573		ILE A		2.724	41.288	52.449	1.00 23.23
5		1574	N	ALA A		7.445			
, ,	ATOM						44.813	53.197	1.00 39.14
	MOTA	1575	CA	ALA A		7.840	46.150	53.611	1.00 37.03
	MOTA	1576	C	ALA A		7.819	47.159	52.482	1.00 34.32
	ATOM	1577	0	ALA A		8.060	46.836	51.311	1.00 30.63
	MOTA	1578	CB	ALA A	203	9.180	46.143	54.309	1.00 38.22
10	MOTA	1579	N	LEU A	204	7.514	48.388	52.910	1.00 33.64
	ATOM	1580	CA	LEU A	204	7.388	49.604	52.102	1.00 32.56
	ATOM	1581	С	LEU A	204	7.993	50.817	52.812	1.00 37.69
	ATOM	1582	0	LEU A		7.854	51.037	54.034	1.00 32.66
	ATOM	1583	СВ	LEU A		5.906	49.929	51.718	1.00 29.74
15	ATOM	1584	CG	LEU A		5.706	51.182		
10		1585		LEU A				50.855	1.00 29.64
	ATOM					6.263	50.994	49.445	1.00 29.47
	MOTA	1586		LEU A		4.222	51.515	50.750	1.00 33.50
	ATOM	1587	N	VAL A		8.670	51.603	51.991	1.00 36.87
20	ATOM	1588	CA	VAL A		9.305	52.821	52.415	1.00 35.15
20	MOTA	1589	С	VAL A	205	9.224	53.795	51.284	1.00 38.41
्रम् इस्त्र	ATOM	1590	0	VAL A	205	9.575	53.462	50.148	1.00 39.50
W.	ATOM	1591	CB	VAL A	205	10.769	52.651	52.804	1.00 36.06
jula.	ATOM	1592		VAL A		11.466	51.794	51.757	1.00 35.08
12 m	ATOM	1593		VAL A		11.432	54.020	52.833	1.00 35.98
25	ATOM	1594	N	VAL A		8.750			
							54.983	51.623	1.00 33.54
UT	ATOM	1595	CA	VAL A		8.623	56.104	50.687	1.00 31.81
John .	ATOM	1596	С	VAL A		9.300	57.343	51.249	1.00 31.62
₩	MOTA	1597	0	VAL A		9.076	57.722	52.406	1.00 34.81
	ATOM	1598	CB	VAL A	206	7.179	56.405	50.305	1.00 33.35
30	ATOM	1599	CG1	VAL A	206	7.129	57.243	49.029	1.00 33.44
	ATOM	1600	CG2	VAL A	206	6.452	55.084	50.109	1.00 31.98
n.	ATOM	1601	N	GLY A		10.130	57.959	50.431	1.00 24.94
	ATOM	1602	CA	GLY A		10.807	59.168	50.861	1.00 27.25
22 Hz	ATOM	1603	С	GLY A		11.802	59.632	49.838	1.00 38.81
35	ATOM	1604	ŏ	GLY A		12.046	58.966	48.840	1.00 30.01
P# 20	ATOM	1605	N	ALA A		12.375	60.783		
		1606						50.113	1.00 41.07
	ATOM		CA	ALA A		13.370	61.354	49.233	1.00 42.72
	MOTA	1607	C	ALA A		14.660	60.550	49.356	1.00 49.10
40	ATOM	1608	0	ALA A		15.651	60.997	49.957	1.00 51.30
40	ATOM	1609	CB	ALA A		13.605	62.810	49.589	1.00 42.95
	ATOM	1610	N	LEU A	209	14.623	59.350	48.773	1.00 40.92
	ATOM	1611	CA	LEU A	209	15.739	58.440	48.825	1.00 39.55
	ATOM	1612	С	LEU A	209	16.756	58.575	47.743	1.00 47.96
	ATOM	1613	0	LEU A	209	16.420	58.843	46.597	1.00 49.44
45	ATOM	1614	CB	LEU A		15.269	56,994	48.894	1.00 37.97
	ATOM	1615	CG	LEU A		14.420	56.803	50.129	1.00 40.46
	ATOM	1616		LEU A		13.713	55.469	50.075	1.00 36.99
	ATOM	1617		LEU A		15.283	56.921	51.387	1.00 33.33
	ATOM	1618	N	GLU A		17.999	58.317	48.182	
50									1.00 42.68
20	ATOM	1619	CA	GLU A		19.205	58.311	47.381	1.00 40.30
	ATOM	1620	С	GLU A		19.965	57.056	47.693	1.00 47.51
	ATOM	1621	0	GLU A		19.708	56.432	48.721	1.00 47.89
	ATOM	1622	CB	GLU A		20.084	59.553	47.613	1.00 42.01
	ATOM	1623	CG	GLU A		19.699	60.734	46.697	1.00 58.26
55	MOTA	1624	CD	GLU A	210	20.524	61.970	46.897	1.00100.00
	ATOM	1625	OE1	GLU A	210	21.629	61.968	47.451	1.00 95.26
	ATOM	1626		GLU A		19.935	63.047	46.486	1.00100.00
	ATOM	1627	N	SER A		20.895	56.662	46.805	1.00100.00
	ATOM	1628	CA	SER A		21.661	55.442		
60			C					47.013	1.00 42.25
00	ATOM	1629		SER A		23.143	55.535	46.667	1.00 43.37
	ATOM	1630	0	SER A		23.649	56.493	46.086	1.00 46.43
	ATOM	1631	CB	SER A		21.025	54.233	46.346	1.00 44.33
	ATOM	1632	OG	SER A		21.274	54.244	44.934	1.00 54.15
	ATOM	1633	N	ARG A	212	23.829	54.497	47.053	1.00 34.85

	ATOM	1634	CA	ARG A 212	25.229	54.328	46.791	1.00	35.41
	ATOM	1635	С	ARG A 212	25.430	52.838	46.567	1.00	45.39
	ATOM	1636	0	ARG A 212	24.840	52.027	47.276	1.00	48.85
	ATOM	1637	CB	ARG A 212	26.101	54.846	47.915	1.00	37.25
5	ATOM	1638	CG	ARG A 212	27.151	55.827	47.402	1.00	
	ATOM	1639	CD	ARG A 212	26.532	56.962	46.587	1.00	
	ATOM	1640	NE	ARG A 212	26.695	58.307	47.148	1.00	
	ATOM	1641	CZ	ARG A 212	25.845	59.301	46.867	1.00	
	ATOM	1642		ARG A 212	24.806	59.105	46.059	1.00	
10	ATOM	1643		ARG A 212	26.032	60.516	47.392	1.00	
•	ATOM	1644	N	GLN A 213	26.210	52.442	45.567	1.00	
	ATOM	1645	CA	GLN A 213	26.408	51.021	45.331	1.00	
	MOTA	1646	C	GLN A 213	27.646	50.537	46.050	1.00	
	ATOM	1647	Ö	GLN A 213	28.740	50.981	45.741	1.00	
15	ATOM	1648	CB	GLN A 213	26.545	50.741	43.846	1.00	
1.7	ATOM	1649	CG	GLN A 213	26.976	49.296	43.532	1.00	
	ATOM	1650	CD	GLN A 213	26.292	48.743	42.301	1.00	
	ATOM	1651		GLN A 213	26.275	47.523	42.102	1.00	
30	MOTA	1652	NE2		25.700	49.618	41.489	1.00	
20	ATOM	1653	N	ILE A 214	27.495	49.649	47.013	1.00	
14 14 14 14 14 14 14 14 14 14 14 14 14 1	ATOM	1654	CA	ILE A 214	28.663	49.206	47.743	1.00	
	MOTA	1655	С	ILE A 214	28.911	47.765	47.536	1.00	
lella.	ATOM	1656	0	ILE A 214	29.726	47.162	48.230	1.00	
14 AV	ATOM	1657	CB	ILE A 214	28.546	49,428	49.250	1.00	35.72
25	MOTA	1658		ILE A 214	27.395	48.573	49.791	1.00	36.13
Ü	ATOM	1659		ILE A 214	28.344	50.911	49.598	1.00	35.79
1.4.	ATOM	1660	CD1	ILE A 214	27.067	48.841	51.260	1.00	46.69
HA.	MOTA	1661	N	GLY A 215	28.199	47.197	46.598	1.00	35.02
#-	ATOM	1662	CA	GLY A 215	28.638	45.855	46.234	1.00	34.88
-30	MOTA	1663	С	GLY A 215	27.970	45.405	44.950	1.00	41.09
7.4	MOTA	1664	0	GLY A 215	27.083	46.048	44.425	1.00	44.25
T.	ATOM	1665	N	PRO A 216	28.448	44.262	44.410	1.00	39.62
	ATOM	1666	CA	PRO A 216	27.890	43.720	43.197	1.00	39.69
ALC: NO.	MOTA	1667	С	PRO A 216	26.369	43.661	43.253	1.00	41.56
35	ATOM	1668	0	PRO A 216	25.655	43.817	42.240	1.00	44.35
Ha site	MOTA	1669	CB	PRO A 216	28.448	42.311	42.996	1.00	39.91
	MOTA	1670	CG	PRO A 216	29.377	41.993	44.164	1.00	41.54
	ATOM	1671	CD	PRO A 216	29.514	43.411	44.897	1.00	37.70
	MOTA	1672	N	ARG A 217	25.846	43.398	44.477	1.00	31.04
40	MOTA	1673	CA	ARG A 217	24.421	43.328	44.652	1.00	29.22
	ATOM	1674	С	ARG A 217	23.928	44.109	45.872	1.00	
	ATOM	1675	0	ARG A 217	22.861	43.885	46.368	1.00	
	MOTA	1676	CB	ARG A 217	24.012	41.844	44.790	1.00	
	ATOM	1677	CG	ARG A 217	25.221	40.963	45.109	1.00	
45	ATOM	1678	CD	ARG A 217	24.828	39.774	45.985		34.08
	MOTA	1679	NE	ARG A 217	26.020	39.183	46.581		45.20
	ATOM	1680	CZ	ARG A 217	25.955	37.894	46.911		65.13
	ATOM	1681		ARG A 217	24.832	37.220	46.716		42.40
	MOTA	1682		ARG A 217		37.300	47.472		48.08
50	ATOM	1683	N	THR A 218		45.022	46.404		31.00
	ATOM	1684	CA	THR A 218		45.886	47.487		31.00
	MOTA	1685	С	THR A 218		47.319	47.021		43.60
	ATOM	1686	ō	THR A 218		47.930	46.512		48.42
	ATOM	1687	СВ	THR A 218		45.845	48.640		36.95
55	ATOM	1688		THR A 218		44.517	49.139		45.66
	ATOM	1689		THR A 218		46.751	49.766		34.17
	ATOM	1690	N	LEU A 219		48.018	47.431		
	MOTA	1691	CA	LEU A 219		49.452			39.19
	ATOM	1691	CA	LEU A 219			47.315		38.18
60	MOTA	1693	0	LEU A 219			48.695		42.32
- 00						49.289	49.498		43.67
	ATOM	1694	CB	LEU A 219		49.841	46.356		37.05
	ATOM	1695	CG CD1	LEU A 219		50.657	45.168		39.31
	ATOM	1696		LEU A 219			44.613	1.00	40.57
	MOTA	1697	CD2	LEU A 219	21.283	50.619	44.131	T-00	29.39

	ATOM	1698	N	VAL A	220	23.066	51.241	48.976	1.00 35.01
	ATOM	1699	CA	VAL A		22.741	51.830	50.253	1.00 36.98
	ATOM	1700	С	VAL A		21.736	52.923	50.043	1.00 44.08
_ *	ATOM	1701	0	VAL A	220	21.959	53.835	49.256	1.00 46.60
5	ATOM	1702	CB	VAL A		23.965	52.346	51.028	1.00 44.95
	ATOM	1703		VAL A		23.675	52.428	52.516	1.00 43.16
	MOTA	1704		VAL A		25.138	51.382	50.828	1.00 47.70
	MOTA	1705	N	TRP A		20.622	52.818	50.731	1.00 41.98
	MOTA	1706	CA	TRP A		19.605	53.828	50.602	1.00 41.64
10	MOTA	1707	С	TRP A		19.464	54.612	51.872	1.00 42.40
	MOTA	1708	0	TRP A		19.461	54.060	52.960	1.00 45.56
	ATOM	1709	CB	TRP A		18.256	53.245	50.186	1.00 41.24
	ATOM	1710	CG	TRP F		18.353	52.459	48.918	1.00 42.59
1.5	ATOM	1711		TRP F		18.888	51.225	48.793	1.00 45.35
15	ATOM	1712		TRP F		17.949	52.873	47.590	1.00 41.62
	ATOM	1713		TRP A		18.826	50.832	47.478	1.00 44.74
	MOTA	1714	CE2			18.243	51.821	46.720	1.00 45.31
.220	MOTA	1715		TRP F		17.345	54.009	47.061	1.00 41.17
	ATOM	1716		TRP A		17.958	51.902	45.346	1.00 42.60
13 20	ATOM	1717	CZ3	TRP F		17.054	54.083	45.710	1.00 39.08
uil	ATOM	1718	CH2	TRP F		17.360	53.040	44.864	1.00 38.48
1 - 5x	ATOM	1719	N	SER A		19.271	55.896	51.688	1.00 37.01
144 144	ATOM	1720	CA	SER A		19.017	56.846	52.748	1.00 38.05
25	ATOM	1721	C	SER A		18.853	58.251	52.205	1.00 45.28
25	MOTA	1722	0	SER A		19.005	58.503	51.008	1.00 44.02
W ()	ATOM	1723	CB	SER A		20.098	56.816	53.820	1.00 39.07
ļ-L	ATOM	1724	OG	SER A		21.322	57.149	53.229	1.00 42.36
18	ATOM	1725	N	GLU A		18.586	59.190	53.088	1.00 40.91
30	ATOM	1726	CA	GLU A		18.465	60.527	52.584	1.00 41.97
30	ATOM	1727	c	GLU A		19.843	61.042	52.234	1.00 50.17
N	ATOM	1728	0	GLU A		20.829	60.701	52.863	1.00 52.02
	ATOM	1729 1730	CB	GLU A		17.856	61.483	53.597	1.00 43.06
	ATOM		CG	GLU A		16.364	61.262	53.861	1.00 51.71
35	ATOM	1731	CD OE1	GLU A		15.799	62.478	54.545	1.00 84.51
	ATOM	1732 1733	OE2			15.905	63.610	54.085	1.00 56.82
	ATOM ATOM	1734	N N	GLU A		15.244	62.222	55.705	1.00 88.87
	ATOM	1735	CA	LYS A		19.892 21.139	61.875	51.229	1.00 47.39
	ATOM	1736	C	LYS A		22.163	62.456 62.683	50.792 51.930	1.00 48.51 1.00 50.90
40	ATOM	1737	Ö	LYS A		23.382	62.569	51.736	1.00 50.90
	ATOM	1738	CB	LYS A		20.843	63.736	49.986	1.00 51.58
	ATOM	1739	CG	LYS A		22.039	64.648	49.723	1.00 31.38
	ATOM	1740	CD	LYS A		21.954	65.397	48.392	1.00 97.82
	ATOM	1741	CE	LYS A		21.646	66.891	48.530	1.00100.00
45	MOTA	1742	NZ	LYS A		22.056	67,700	47.362	1.00100.00
	MOTA	1743	N	GLU A		21.683	63.011	53.123	1.00 45.77
	ATOM	1744	CA	GLU A		22.607	63.309	54.199	1.00 46.00
	ATOM	1745	С	GLU A		23.227	62.150	54.902	1.00 47.99
	ATOM	1746	0	GLU A		24.107	62.354	55.732	1.00 47.21
50	ATOM	1747	CB	GLU A		22.057	64.296	55.210	1.00 47.71
	ATOM	1748	CG	GLU A		20.530	64.296	55.182	1.00 63.24
	ATOM	1749	CD	GLU A		19.931	65.219	54.150	1.00 75.13
	MOTA	1750	OE1	GLU A	225	20.187	66.420	54.046	1.00 54.64
*	MOTA	1751	OE2	GLU A	225	19.039	64.578	53.420	1.00 49.64
55	MOTA	1752	N	GLN A	226	22,798	60.949	54.564	1.00 43.92
	ATOM	1753	CA	GLN A		23.340	59.772	55.224	1.00 43.91
	ATOM	1754	С	GLN A	226	24.036	58.756	54.322	1.00 45.86
	ATOM	1755	0	GLN A		24.756	57.871	54.806	1.00 45.70
	ATOM	1756	CB	GLN A		22.252	59.084	56.063	1.00 45.27
60	ATOM	1757	CG	GLN A		21.965	59.790	57.400	1.00 31.17
	ATOM	1758	CD		226	21.297	61.155	57.302	1.00 44.48
	MOTA	1759		GLN A		21.823	62.149	57.820	1.00 37.36
	MOTA	1760		GLN A		20.115	61.202	56.696	1.00 30.28
	MOTA	1761	N	VAL A	227	23.814	58.871	53.021	1.00 41.20

	MOTA	1762	CA	VAL A	227	24.406	57.947	52.071	1.00 43.13
	MOTA	1763	С	VAL A		25.884	57.670	52.261	1.00 50.55
	MOTA	1764	0	VAL A	227	26.298	56.518	52.480	1.00 53.01
	ATOM	1765	CB	VAL A	227	24.155	58.293	50.604	1.00 49.39
5	ATOM	1766		VAL A		24.319	57.029	49.771	
, ,									1.00 48.89
	ATOM	1767	CG2	VAL A	227	22.752	58.851	50.421	1.00 50.47
	ATOM	1768	N	GLU A	228	26.696	58.718	52.170	1.00 44.08
	ATOM	1769	CA	GLU A		28.123	58.542	52.310	1.00 41.71
10	MOTA	1770	С	GLU A		28.514	57.871	53.583	1.00 44.20
10	MOTA	1771	0	GLU A	228	29.227	56.868	53.589	1.00 44.88
	ATOM	1772	CB	GLU A	228	28.935	59.824	52.102	1.00 43.08
		1773	ĊĠ	GLU A					
	MOTA					29.153	60.161	50.611	1.00 64.74
	MOTA	1774	$^{\rm CD}$	GLU A	228	29.114	58.965	49.701	1.00 84.29
	ATOM	1775	OE1	GLU A	228	29.975	58.107	49.685	1.00 84.36
15	ATOM	1776	OE2			28.064	58.951		
15								48.917	1.00 73.81
	ATOM	1777	N	LYS A	229	28.066	58.423	54.685	1.00 39.79
	ATOM	1778	CA	LYS A	229	28.449	57.796	55.922	1.00 39.04
	ATOM	1779	С	LYS A		27.949	56.375	55.930	1.00 40.38
.200 BB.									
20	MOTA	1780	0	LYS A		28.639	55.433	56.346	1.00 43.63
20	ATOM	1781	CB	LYS A	229	28.129	58.585	57.187	1.00 39.79
43 Mar	MOTA	1782	CG	LYS A	229	28.903	58.072	58.394	1.00 63.75
41	ATOM			LYS A					
ha da		1783	CD			28.498	58.763	59.685	1.00 77.46
E 200	ATOM	1784	ÇE	LYS A	229	29.677	59.084	60.593	1.00 94.73
ud inc	ATOM	1785	NZ	LYS A	229	30.344	60.353	60.256	1.00100.00
25	ATOM	1786	N	SER A		26.741	56.220	55.428	
0 3301									1.00 28.48
	MOTA	1787	CA	SER A		26.174	54.891	55.377	1.00 25.93
##x	ATOM	1788	С	SER A	230	27.089	53.988	54.587	1.00 30.26
	MOTA	1789	0	SER A		27.469	52.855	54.955	1.00 28.48
康.									
30	MOTA	1790	CB	SER A		24.824	54.927	54.694	1.00 30.08
30	MOTA	1791	OG	SER A	230	23.822	55.293	55.605	1.00 41.60
	MOTA	1792	N	ALA A	231	27.436	54.536	53.459	1.00 31.13
13	ATOM	1793	CA	ALA A		28.288	53.820	52.593	
tank									1.00 36.66
de m	MOTA	1794	С	ALA A		29.597	53.383	53.270	1.00 47.68
<u> </u>	MOTA	1795	0	ALA A	231	30.003	52.238	53.103	1.00 54.59
35	ATOM	1796	CB	ALA A	231	28.406	54.518	51.257	1.00 38.49
Ha sad	ATOM	1797	N	TYR A		30.256	54.246	54.060	
									1.00 40.77
	ATOM	1798	CA	TYR A		31.500	53.830	54.730	1.00 38.40
	ATOM	1799	С	TYR A	232	31.265	52.721	55.753	1.00 39.70
	MOTA	1800	0	TYR A	232	32.041	51.772	55.862	1.00 36.46
40	ATOM	1801	СВ	TYR A		32.311		55.414	
							54.981		1.00 38.27
	MOTA	1802	CG	TYR A		33.497	54.525	56.303	1.00 42.36
	ATOM	1803	CD1	TYR A	232	34.755	54.238	55.753	1.00 46.41
	ATOM	1804	CD2	TYR A	232	33.373	54.394	57.691	1.00 40.99
	ATOM	1805		TYR A					
AE						35.835	53.815	56.534	1.00 47.23
45	ATOM	1806		TYR A		34.441	53.979	58.496	1.00 40.10
	ATOM	1807	CZ	TYR A	232	35.680	53.695	57.916	1.00 48.59
	ATOM	1808	OH	TYR A		36.734	53.282	58.698	1.00 51.92
	ATOM	1809	N	GLU A					
						30.191	52.883	56.519	1.00 35.75
60	MOTA	1810	CA	GLU A	233	29.835	51.984	57.606	1.00 34.55
50	MOTA	1811	С	GLU A	233	29.633	50.498	57.252	1.00 38.39
	ATOM	1812	0	GLU A		30.152	49.576	57.892	1.00 38.55
	ATOM	1813	CB	GLU A		28.673	52.623	58.414	1.00 34.48
	ATOM	1814	CG	GLU A	233	28.666	52.262	59.912	1.00 24.95
	MOTA	1815	CD	GLU A	233	29.463	53.183	60.787	1.00 37.55
55									
	ATOM	1816		GLU A		29.408	54.410	60.741	1.00 55.33
	ATOM	1817	OE2	GLU A	233	30.216	52.518	61.619	1.00 40.65
	MOTA	1818	N	PHE A	234	28.867	50.282	56.202	1.00 33.02
	MOTA	1819	CA	PHE A		28.493	48.974	55.719	1.00 29.90
C 0	MOTA	1820	С	PHE A		29.341	48.398	54.592	1.00 34.69
60	MOTA	1821	0	PHE A	234	28.883	47.521	53.823	1.00 34.21
	ATOM	1822	CB	PHE A	234	27.020	49.081	55.293	1.00 30.23
	ATOM	1823	CG	PHE A		26.215	49.752	56.394	
									1.00 30.32
	ATOM	1824		PHE A		26.518	49,521	5 7. 739	1.00 31.50
	ATOM	1825	CD2	PHE A	234	25.151	50.605	56.102	1.00 28.66

	ATOM	1826	CE1	PHE A	234	25.780	50.103	58.772	1.00 30.43
	ATOM	1827	CE2	PHE A		24.407	51.203	57.121	1.00 29.60
	ATOM	1828	CZ	PHE A		24.725	50.959	58.458	
									1.00 27.47
5	ATOM	1829	N	SER A		30.571	48.874	54.476	1.00 29.55
, ,	MOTA	1830	CA	SER A		31.428	48.366	53.412	1.00 28.64
	ATOM	1831	С	SER A		31.387	46.858	53.338	1.00 30.38
	MOTA	1832	0	SER A		31.166	46.252	52.282	1.00 32.37
	MOTA	1833	CB	SER A		32.861	48.787	53.604	1.00 31.15
1	ATOM	1834	OG	SER A		33.028	49.368	54.873	1.00 39.32
10	MOTA	1835	N	GLU A	236	31.698	46.299	54.504	1.00 22.49
	ATOM	1836	CA	GLU A	236	31.815	44.873	54.737	1.00 23.79
	MOTA	1837	C	GLU A	236	30.627	43.992	54.380	1.00 32.37
	MOTA	1838	0	GLU A	236	30.697	42.772	54.545	1.00 29.91
	MOTA	1839	CB	GLU A		32.305	44.529	56.134	1.00 24.06
15	ATOM	1840	CG	GLU A		33.491	45.403	56.585	1.00 22.96
	ATOM	1841	CD	GLU A		33.600	45.492	58.090	1.00 22.30
	ATOM	1842	OE1	GLU A			45.482		1.00 37.01
		1843	OE2	GLU A		32.633		58.849	
.47 49,	ATOM					34.848	45.518	58.494	1.00 78.68
20	ATOM	1844	N	THR A		29.560	44.593	53.891	1.00 34.11
20	ATOM	1845	CA	THR A		28.384	43.823	53.539	1.00 33.69
	ATOM	1846	С	THR A		28.644	42.609	52.644	1.00 33.33
jalis	MOTA	1847	0	THR A		28.517	41.451	53.048	1.00 31.09
	ATOM	1848	CB	THR A		27.218	44.710	53.057	1.00 37.99
SHA	ATOM	1849	OG1	THR A	237	26.899	45.675	54.048	1.00 33.49
25	ATOM	1850	CG2	THR A	237	25,995	43.862	52.744	1.00 25.66
	ATOM	1851	N	GLU A	238	29.020	42.854	51.409	1.00 29.69
# # # # # # # # # # # # # # # # # # #	ATOM	1852	CA	GLU P	238	29.267	41.734	50.520	1.00 27.05
	ATOM	1853	С	GLU A	238	30.071	40.638	51.146	1.00 33.17
# 1 .	ATOM	1854	0	GLU A	238	29.660	39.497	51.055	1.00 38.50
30	MOTA	1855	CB	GLU P		29.851	42.080	49.161	1.00 27.50
17	MOTA	1856	CG	GLU A		30.116	40.813	48.320	1.00 18.83
NJ	ATOM	1857	CD	GLU A		28.902	40.297	47.596	1.00 41.67
	ATOM	1858	OE1	GLU A		27.848	40.909	47.464	1.00 33.59
	ATOM	1859	OE2	GLU P		29.085	39.089	47.138	1.00 46.30
35	ATOM	1860	N	SER A		31.203	40.973	51.772	1.00 24.44
Ba and	ATOM	1861	CA	SER A		32.045	39.957	52.387	1.00 24.60
	ATOM	1862	С	SER A		31.245	39.060	53.344	1.00 35.72
	ATOM	1863	0	SER A		31.379	37.830	53.360	1.00 35.25
	ATOM	1864	CB	SER A		33.231	40.601	53.074	1.00 29.14
40	ATOM	1865	OG	SER A		32.747	41.590	53.961	1.00 54.60
	ATOM	1866	N	MET A		30.382	39.703	54.154	1.00 34.00
	MOTA	1867	CA	MET A		29.529	38.993	55.091	1.00 33.13
	ATOM	1868	C	MET A		28.603			
		1869	0				38.075	54.325	1.00 35.65
45	ATOM			MET A		28.435	36.926	54.689	1.00 35.99
7.7	ATOM	1870	CB	MET A		28.736	39.945	55.993	1.00 26.50
	ATOM	1871	CG	MET A		29.691	40.675	56.910	1.00 27.57
	ATOM	1872	SD	MET A		28.871	41.986	57.833	1.00 32.91
	MOTA	1873	CE	MET A		30.040	42.085	59.183	1.00 28.47
50	MOTA	1874	N	LEU F		28.019	38.603	53.243	1.00 32.77
50	MOTA	1875	CA	LEU A		27.120	37.859	52.381	1.00 29.87
	MOTA	1876	С	LEU F		27.848	36.615	51.878	1.00 36.76
	ATOM	1877	0	LEU A		27.302	35.509	51.858	1.00 36.97
	ATOM	1878	CB	LEU A		26.715	38.753	51.196	1.00 29.71
**±_	ATOM	1879	CG	LEU F	241	25.283	39.289	51.237	1.00 37.68
55	ATOM	1880	CD1	LEU A	241	25.174	40.552	50.389	1.00 35.76
	ATOM	1881	CD2	LEU F	241	24.309	38.257	50.673	1.00 45.60
	ATOM	1882	N	LYS A		29.114	36.806	51.468	1.00 34.76
	ATOM	1883	CA	LYS A		29.908	35.702	50.972	1.00 33.62
	ATOM	1884	c	LYS A		30.072	34.690	52.039	1.00 33.02
60	ATOM	1885	Ö	LYS A		29.887	33.512	51.795	1.00 32.10
_ -	ATOM	1886	CB	LYS A		31.292	36.069	50.468	1.00 32.36
	ATOM	1887	CG	LYS A		31.406	36.263	48.961	1.00 38.43
	ATOM	1888	CD	LYS A		31.160			
	ATOM	1889	CE	LYS A			37.721	48.536	1.00 88.36
	ALI OF	1009	CE	PIO V	1 242	32.371	38.456	47.943	1.00100.00

WO 00/50577

PCT/SE00/00384

32.033 39.411 46.862 1.00100.00 MOTA 1890 NZLYS A 242 1891 N ILE A 243 30.428 35.154 53.227 1.00 30.87 ATOM 54.359 54.764 1.00 31.70 1.00 36.50 ATOM CA ILE A 243 30.627 34.229 1892 ILE A 243 33.458 1893 С 29.381 ATOM 55.119 5 32.303 1.00 39.33 ILE A 243 29.458 ATOM 1894 0 1.00 32.36 ILE A 243 34.886 55.579 1895 31.227 CB ATOM 1896 CG1 ILE A 243 32.630 35.337 55.222 1.00 32.09 ATOM 33.891 56.718 MOTA 1897 CG2 ILE A 243 31.243 1.00 28.26 CD1 ILE A 243 33.035 36.578 55.981 1898 1.00 20.09 ATOM ALA A 244 34.120 33.519 10 ATOM 1899 N 28.237 54.708 1.00 32.10 26.968 1900 CA ALA A 244 55.066 1.00 32.95 MOTA ALA A 244 32.392 26.600 54.127 1.00 36.35 ATOM 1901 С ALA A 244 26.074 31.358 1.00 36.88 ATOM 1902 0 54.546 34.576 1903 CB ALA A 244 25.858 55.123 1.00 34.02 MOTA 15 ATOM 1904 N **GLU A 245** 26.890 32.617 52.846 1.00 31.20 ATOM 1905 CA GLU A 245 26.614 31.635 51.818 1.00 29.26 27.360 26.849 26.908 GLU A 245 30.354 52.092 1906 С 1.00 35.18 MOTA GLU A 245 1907 29.276 51.800 1.00 36.21 ATOM 0 26.908 25.701 26.026 1908 GLU A 245 32.177 50.421 ATOM CB 1.00 30.22 GLU A 245 20 ATOM 1909 CG 32.938 49.842 1.00 39.79 CD GLU A 245 33.564 1910 48.529 1.00 51.91 Barre B. ATOM OE1 GLU A 245 26.945 1.00 34.19 34.351 48.358 ATOM 1911 1 OE2 GLU A 245 25.246 ATOM 1912 33.142 47.585 1.00 47.48 1 ATOM 1913 ASP A 246 28.570 30.484 52.680 1.00 32.29 N ATOM 1914 CA ASP A 246 29.417 29.350 53.033 1.00 30.70 ATOM 1915 С ASP A 246 28.848 28.645 54.230 1.00 35.47 ASP A 246 28.881 27.417 ATOM 1916 54.347 0 1.00 37.08 30.873 1 ASP A 246 29.717 ATOM 1917 CB 53.355 1.00 33.17 28.473 27.789 ASP A 246 1.00 64.49 MOTA 1918 31.709 53.413 CG **30** OD1 ASP A 246 52.437 1.00 67.15 1.00 79.01 ATOM 1919 31.934 OD2 ASP A 246 28.167 54.622 ATOM 1920 32.118 1.00 33.59 LEU A 247 MOTA 1921 N 28.323 29.434 55.134 The state of ATOM 1922 CA LEU A 247 27.731 28.868 56.334 1.00 36.70 ATOM 1923 LEU A 247 26.355 28.208 56.083 C 1.00 35.92 **...35** LEU A 247 26.060 27.110 56.551 MOTA 1924 0 1.00 30.77 LEU A 247 LEU A 247 27.562 28.732 ATOM 1925 CB 29.954 57.435 1.00 38.34 MOTA 1926 30.100 58.394 1.00 44.30 CG CD1 LEU A 247 29.341 29.779 28.738 1.00 48.20 MOTA 1927 58.641 1.00 35.25 CD2 LEU A 247 31.013 57.815 **ATOM** 1928 40 GLY A 248 25.471 28.887 55.353 1.00 34.97 MOTA 1929 N 1.00 36.00 MOTA 1930 CA **GLY A 248** 24.160 28.315 55.181 MOTA 1931 **GLY A 248** 23.754 27.976 53.778 1.00 37.99 GLY A 248 22.637 53.526 ATOM 1932 0 27.524 1.00 38.13 MOTA 1933 N GLY A 249 24.637 28.158 52.849 1.00 30.74 45 GLY A 249 GLY A 249 ATOM 1934 CA 24.203 27.852 51.526 1.00 30.15 50.759 1.00 38.91 ATOM 1935 С 23.918 29.131 MOTA GLY A 249 24.126 30.240 51.238 1936 0 1.00 41.32 PRO A 250 ATOM 1937 23.453 28.946 49.547 1.00 38.93 N ATOM 1938 PRO A 250 23.173 30.021 CA 48.639 1.00 38.03 50 MOTA 1939 С PRO A 250 22.203 31.078 49.096 1.00 42.17 21.258 ATOM 1940 0 PRO A 250 30.823 49.840 1.00 45.20 PRO A 250 ATOM 1941 CB 22.663 29.357 47.352 1.00 39.18 MOTA 1942 CG PRO A 250 22.952 27.864 47.436 1.00 41.01 PRO A 250 1.00 38.57 1.00 35.37 1943 ATOM CD 23.396 27.610 48.865 55 1944 TYR A 251 22.486 32.275 48.600 ATOM N TYR A 251 1.00 34.87 MOTA 1945 CA 21.692 33.461 48.817 MOTA 1946 TYR A 251 20.740 47.649 1.00 39.55 С 33.479 ATOM 1947 TYR A 251 21.125 33.794 46.535 1.00 42.57 0 TYR A 251 1948 48.790 MOTA CB 22.540 34.759 1.00 35.07 60 21.711 49.119 MOTA TYR A 251 1949 CG 35.980 1.00 35.25 ATOM 1950 CD1 TYR A 251 21.341 36.229 50.441 1.00 33.14 36.846 MOTA 1951 CD2 TYR A 251 21.260 48.121 1.00 37.98 CE1 TYR A 251 1952 20.575 50.781 MOTA 37.341 1.00 28.05 MOTA 1953 CE2 TYR A 251 20.492 37.967 48.443 1.00 40.05

	ATOM	1954	cz	TYR A 251	20.160	38.213	49.777	1.00 42.84
	ATOM	1955	ОН	TYR A 251	19.409	39.307	50.112	1.00 39.70
	ATOM	1956	N	VAL A 252	19.510	33.102	47.914	1.00 32.21
	ATOM	1957	CA	VAL A 252	18.495	33.003	46.899	1.00 30.05
5	ATOM	1958	С	VAL A 252	17.708	34.279	46.631	1.00 38.47
	MOTA	1959	0	VAL A 252	17.000	34.340	45.640	1.00 40.65
	MOTA	1960	CB	VAL A 252	17.560	31.845	47.253	1.00 31.27
	ATOM	1961	CG1	VAL A 252	18.378	30.605	47.643	1.00 28.15
	ATOM	1962	CG2	VAL A 252	16.614	32.234	48.405	1.00 30.93
10	ATOM	1963	N	TRP A 253	17.800	35.292	47.504	1.00 32.44
	ATOM	1964	CA	TRP A 253	17.041	36.509	47.309	1.00 30.93
	ATOM	1965	С	TRP A 253	17.468	37.341	46.119	1.00 43.56
	MOTA	1966	0	TRP A 253	16.690	38.119	45.568	1.00 46.70
15	MOTA	1967	CB	TRP A 253	16.898	37.302	48.606	1.00 29.65
15	ATOM	1968	CG CD1	TRP A 253	16.364	36.369	49.625	1.00 30.19
	ATOM	1969		TRP A 253	17.086	35.546	50.413	1.00 32.81
	ATOM ATOM	1970 1971		TRP A 253	14.989 16.251	36.110 34.794	49.913	1.00 29.63
	ATOM	1972	CE2		14.955	35.128	51.194 50.912	1.00 30.69
20	ATOM	1973		TRP A 253	13.789	36.637	49.450	1.00 31.50 1.00 30.18
13 20	ATOM	1974		TRP A 253	13.746	34.657	51.433	1.00 30.18
12.00	ATOM	1975	CZ3		12.600	36.164	49.958	1.00 30.31
i i	ATOM	1976	CH2		12.579	35.176	50.946	1.00 31.14
3 PX	ATOM	1977	N	GLY A 254	18.697	37.182	45.675	1.00 42.35
25	ATOM	1978	CA	GLY A 254	19.101	37.944	44.509	1.00 41.34
<u>I</u>	ATOM	1979	С	GLY A 254	19.875	39.192	44.858	1.00 45.47
 - 	ATOM	1980	0	GLY A 254	21.079	39.236	44.671	1.00 45.89
	MOTA	1981	N	GLN A 255	19.160	40.210	45.351	1.00 41.86
#R	MOTA	1982	CA	GLN A 255	19.746	41.488	45.675	1.00 38.67
30	ATOM	1983	С	GLN A 255	19.576	41.776	47.153	1.00 40.18
Tu -	ATOM	1984	0	GLN A 255	18.494	41.811	47.659	1.00 38.67
T.	MOTA	1985	CB	GLN A 255	19.023	42.552	44.836	1.00 37.82
72 T	ATOM	1986	CG	GLN A 255	19.455	43.979	45.169	1.00 50.17
35	ATOM	1987	CD	GLN A 255	20.618	44.368	44.283	1.00 62.88
14.33	ATOM	1988		GLN A 255	21.104	43.612	43.463	1.00 55.76
	MOTA	1989 1990	NE2		21.057	45.625	44.479	1.00 34.97
	ATOM ATOM	1990	N CA	TYR A 256 TYR A 256		41.900 42.361	47.866	1.00 33.01
	ATOM	1992	CA	TYR A 256		43.854	49.258 49.329	1.00 28.69 1.00 26.72
40	ATOM	1993	Õ	TYR A 256		44.321	49.225	1.00 24.22
	ATOM	1994	СВ	TYR A 256		41.629	50.075	1.00 29.99
	MOTA	1995	CG	TYR A 256		41.867	51.556	1.00 35.47
	ATOM	1996	CD1	TYR A 256		41.200	52.250	1.00 35.76
26	MOTA	1997	CD2	TYR A 256	22.405	42.746	52.239	1.00 37.52
45	ATOM	1998	CE1	TYR A 256	20.436	41.396	53.599	1.00 25.80
	ATOM	1999	CE2	TYR A 256		42.946	53.588	1.00 39.10
	ATOM	2000	CZ	TYR A 256		42.275	54.268	1.00 31.78
	MOTA	2001	OH	TYR A 256		42.433	55.631	1.00 37.35
60	MOTA	2002	N	ASP A 257		44.613	49.463	1.00 23.26
<i>5</i> 0	ATOM	2003	CA	ASP A 257		46.027	49.621	1.00 23.47
	ATOM	2004	С	ASP A 257		46.444	51.071	1.00 35.90
	ATOM ATOM	2005 2006	O CB	ASP A 257 ASP A 257		45.661	51.967	1.00 39.48
	ATOM	2007	CG	ASP A 257		46.803	48.758	1.00 24.13
55	ATOM	2007		ASP A 257		47.030 46.675	47.388 47.220	1.00 38.50 1.00 42.61
<i></i>	MOTA	2009		ASP A 257		47.555	46.517	1.00 42.61
	ATOM	2010	N N	LEU A 258		47.661	51.386	1.00 29.02
	ATOM	2011	CA	LEU A 258		48.159	52.735	1.00 30.80
	ATOM	2012	C	LEU A 258		49.466	52.765	1.00 36.37
60	ATOM	2013	ō	LEU A 258		50.302	51.840	1.00 37.98
	ATOM	2014	СВ	LEU A 258		48.442	53.274	1.00 24.71
	MOTA	2015	CG	LEU A 258	22.552	47.191	53.491	1.00 31.13
	MOTA	2016		LEU A 258		47.567	54.043	1.00 30.89
	MOTA	2017	CD2	LEU A 258	21.854	46.282	54.500	1.00 33.65

	MOTA	2018	N	LEU A 259	18.762	49.632	53.838	1.00 29.87
	MOTA	2019	CA	LEU A 259	18.006	50.849	54.052	1.00 28.43
	ATOM	2020	С	LEU A 259	18.283	51.453	55.446	1.00 31.30
_ *	MOTA	2021	0	LEU A 259	18.055	50.819	56.477	1.00 31.19
5	ATOM	2022	CB	LEU A 259	16.500	50.809	53.693	1.00 27.63
	MOTA	2023	CG	LEU A 259	15.706	51.980	54.298	1.00 31.51
	MOTA	2024		LEU A 259	16.026	53.300	53.605	1.00 32.32
	MOTA	2025		LEU A 259	14.212	51.731	54.253	1.00 26.87
10	MOTA	2026	N	VAL A 260	18.807	52.683	55.447	1.00 25.88
10	MOTA	2027	CA	VAL A 260	19.105	53.435	56.638	1.00 25.99
	ATOM	2028	C	VAL A 260	17.896	54.336	56.796	1.00 34.83
	ATOM	2029	O	VAL A 260	17.647	55.187	55.959	1.00 41.92
	ATOM	2030 2031	CB	VAL A 260 VAL A 260	20.390 20.701	54.234 55.179	56.408 57.592	1.00 29.97 1.00 32.08
15	ATOM ATOM	2031		VAL A 260	21.563	53.295	56.130	1.00 32.08
1.7	ATOM	2032	N	LEU A 261	17.098	54.120	57.815	1.00 28.41
	ATOM	2034	CA	LEU A 261	15.865	54.878	58.024	1.00 25.52
	ATOM	2035	C	LEU A 261	16.016	56.054	58.948	1.00 29.42
APP AT	ATOM	2036	0	LEU A 261	17.090	56.300	59.489	1.00 29.96
20	ATOM	2037	СВ	LEU A 261	14.874	53.921	58.706	1.00 25.70
	ATOM	2038	CG	LEU A 261	14.387	52.877	57.740	1.00 33.14
Handa St. 1	ATOM	2039		LEU A 261	15.161	51.571	57.929	1.00 32.73
ļaš,	ATOM	2040		LEU A 261	12.900	52.686	57.935	1.00 43.74
्रमाः सर्वे मार्	ATOM	2041	N	PRO A 262	14.903	56.758	59.142	1.00 28.52
25	MOTA	2042	CA	PRO A 262	14.894	57.870	60.047	1.00 28.50
WT.	ATOM	2043	С	PRO A 262	15.152	57.294	61.432	1.00 35.36
lat.	ATOM	2044	0	PRO A 262	14.866	56.124	61.683	1.00 34.52
*	ATOM	2045	CB	PRO A 262	13.512	58.512	59.971	1.00 29.19
	ATOM	2046	CG	PRO A 262	12.707	57.719	58.964	1.00 34.34
30	ATOM	2047	CD	PRO A 262	13.581	56 .5 75	58.492	1.00 30.63
n. Ma	MOTA	2048	N	PRO A 263	15.706	58.105	62.327	1.00 31.50
i ingg	MOTA	2049	CA	PRO A 263	16.060	57.657	63.673	1.00 28.77
	MOTA	2050	C	PRO A 263	14.966	57.021	64.493	1.00 29.15
	ATOM	2051	0	PRO A 263	15.256	56.335	65.434	1.00 26.36
4.35	ATOM	2052	CB	PRO A 263	16.652	58.867	64.392	1.00 29.16
	ATOM	2053	CG	PRO A 263	16.851	59.954	63.335	1.00 31.55
	MOTA	2054	CD	PRO A 263	15.994	59.558	62.138	1.00 29.17
	ATOM ATOM	2055 2056	N CA	SER A 264 SER A 264	13.712 12.578	57.258 56.703	64.143 64.864	1.00 33.87
40	ATOM	2057	CA	SER A 264	12.403	55.223	64.604	1.00 33.81 1.00 37.36
-10	ATOM	2058	Ö	SER A 264	11.529	54.570	65.201	1.00 37.30
	ATOM	2059	СВ	SER A 264	11.280	57.423	64.576	1.00 35.61
	ATOM	2060	OG	SER A 264	10.955	57.276	63.201	1.00 53.45
	ATOM	2061	N	PHE A 265	13.213	54.684	63.710	1.00 29.00
45	MOTA	2062	CA	PHE A 265	13.136	53.256	63.453	1.00 28.56
	MOTA	2063	С	PHE A 265	13.260	52.491	64.787	1.00 28.49
	ATOM	2064	0	PHE A 265	14.208	52.675	65.533	1.00 27.36
	ATOM	2065	CB	PHE A 265	14.200	52.833	62.454	1.00 31.40
	MOTA	2066	CG	PHE A 265	13.875	51.458	62.028	1.00 34.51
50	ATOM	2067		PHE A 265	12.601	51.174	61.543	1.00 35.11
	MOTA	2068		PHE A 265	14.814	50.435	62.156	1.00 38.94
	ATOM	2069		PHE A 265	12.282	49.876	61.154	1.00 37.42
	ATOM	2070		PHE A 265	14.511	49.131	61.772	1.00 42.65
55	ATOM	2071	CZ	PHE A 265	13.236	48.860	61.274	1.00 40.14
	MOTA MOTA	2072 2073	N CA	PRO A 266 PRO A 266	12.272 12.249	51.650 50.945	65.128 66.419	1.00 24.06
	MOTA	2074	C	PRO A 266	13.231	49.794	66.701	1.00 20.62 1.00 29.34
	ATOM	2075	0	PRO A 266	13.231	49.794	67.847	1.00 29.34
	ATOM	2076	CB	PRO A 266	10.808	50.463	66.593	1.00 28.17
60	ATOM	2077	CG	PRO A 266	10.076	50.686	65.281	1.00 21.07
-,-	ATOM	2078	CD	PRO A 266	11.046	51.355	64.325	1.00 19.44
	MOTA	2079	N	TYR A 267	13.922	49.280	65.676	1.00 27.23
	MOTA	2080	CA	TYR A 267	14.849	48.160	65.817	1.00 25.74
	ATOM	2081	С	TYR A 267	16.181	48.454	65.189	1.00 32.57

	MOTA	2082	0	TYR A 267	16.281	49.316	64.324	1.00 32.48
	MOTA	2083	CB	TYR A 267	14.298	46.903	65.121	1.00 25.07
	MOTA	2084	CG	TYR A 267	12.968	46.502	65.674	1.00 24.45
_	MOTA	2085		TYR A 267	12.915	45.765	66.856	1.00 27.05
5	MOTA	2086		TYR A 267	11.776	46.851	65.037	1.00 22.15
	ATOM	2087		TYR A 267	11.697	45.387	67.419	1.00 25.01
	MOTA	2088		TYR A 267	10.548	46.496	65.596	1.00 19.09
	ATOM	2089	CZ	TYR A 267	10.510	45.767	66.786	1.00 17.98
10	ATOM	2090	OH	TYR A 267	9.302	45.416	67.353	1.00 19.51
10	MOTA	2091	N	GLY A 268	17.196	47.698	65.627	1.00 30.22
	ATOM	2092	CA	GLY A 268	18.547	47.826	65.114	1.00 27.29
	ATOM	2093	C	GLY A 268	18.485	47.620	63.614	1.00 29.82
	ATOM	2094	0	GLY A 268 GLY A 269	19.136 17.637	48.297	62.836	1.00 32.99
15	ATOM	2095 2096	N	GLY A 269	17.393	46.676 46.320	63.228	1.00 23.19
15	ATOM	2090	CA C	GLY A 269	16.187	45.402	61.853 61.777	1.00 21.62
	ATOM	2097	0	GLY A 269	15.681	44.948	62.820	1.00 27.53
	ATOM ATOM	2099	N	MET A 270	15.735	45.154	60.528	1.00 20.14
	ATOM	2100	CA	MET A 270	14.615	44.267	60.176	1.00 27.81 1.00 25.61
20	MOTA	2101	C	MET A 270	14.956	43.585	58.874	1.00 23.61
ul Zu	MOTA	2102	ō	MET A 270	15.221	44.247	57.867	1.00 33.30
jak.	MOTA	2103	CB	MET A 270	13.247	44.936	60.028	1.00 34.07
regard interest	MOTA	2104	CG	MET A 270	12.195	43.937	59.602	1.00 28.81
2200-	MOTA	2105	SD	MET A 270	11.875	42.742	60.929	1.00 20.01
25	ATOM	2106	CE	MET A 270	10.720	41.621	60.082	1.00 35.30
H	ATOM	2107	N	GLU A 271	14.995	42.263	58.904	1.00 32.20
- L	ATOM	2108	CA	GLU A 271	15.393	41.459	57.753	1.00 33.32
#	ATOM	2109	С	GLU A 271	14.419	41.382	56.567	1.00 40.86
1=4 ₁	ATOM	2110	0	GLU A 271	14.087	40.285	56.107	1.00 42.02
1.30	ATOM	2111	CB	GLU A 271	15.802	40.054	58.230	1.00 35.05
	ATOM	2112	CG	GLU A 271	14.607	39.218	58.760	1.00 33.55
	ATOM	2113	CD	GLU A 271	14.291	39.428	60.219	1.00 25.52
	ATOM	2114	OE1		14.586	40.436	60.844	1.00 37.23
in all	ATOM	2115		GLU A 271	13.699	38.393	60.757	1.00 25.86
35	ATOM	2116	N	ASN A 272	13.978	42.535	56.052	1.00 35.34
	ATOM	2117	CA	ASN A 272	13.057	42.544	54.928	1.00 33.26
	ATOM	2118	C	ASN A 272	13.787	42.048	53.702	1.00 34.47
	ATOM	2119	0	ASN A 272	14.811	42.613	53.351	1.00 33.64
40	ATOM	2120	CB	ASN A 272	12.441	43.947	54.719	1.00 30.65
40	ATOM	2121	CG	ASN A 272	11.667	44.453	55.935	1.00 42.50
	ATOM	2122		ASN A 272 ASN A 272	11.908	45.554	56.475	1.00 47.09
	MOTA MOTA	2123 2124	ND2	PRO A 273	10.716 13.281	43.661	56.371	1.00 24.31
	ATOM	2124	CA	PRO A 273	13.201	40.983 40.373	53.078 51.910	1.00 29.63 1.00 28.47
45	ATOM	2126	C	PRO A 273	14.303	41.345	50.819	1.00 20.47
	ATOM	2127	ŏ	PRO A 273	13.457	42.089	50.372	1.00 30.43
	ATOM	2128	ČВ	PRO A 273	12.991	39.305	51.381	1.00 31.03
	ATOM	2129	CG	PRO A 273	11.829	39.237	52.365	1.00 36.65
	ATOM	2130	CD	PRO A 273	11.927	40.440	53.310	1.00 30.84
50	ATOM	2131	N	CYS A 274	15.571	41.333	50.431	1.00 27.40
	ATOM	2132	CA	CYS A 274	16.069	42.206	49.373	1.00 28.17
	ATOM	2133	C	CYS A 274	16.327	43.604	49.860	1.00 27.35
	MOTA	2134	0	CYS A 274	17.114	44.345	49.248	1.00 28.53
	MOTA	2135	CB	CYS A 274	15.121	42.347	48.145	1.00 32.00
55	MOTA	2136	SG	CYS A 274	14.659	40.798	47.340	1.00 38.42
	MOTA	2137	N	LEU A 275	15.658	43.972	50.947	1.00 26.20
	MOTA	2138	CA	LEU A 275	15.789	45.315	51.535	1.00 29.54
	MOTA	2139	С	LEU A 275	15.857	45.279	53.059	1.00 32.52
· .	MOTA	2140	0	LEU A 275	14.859	45.250	53.772	1.00 32.44
60	MOTA	2141	CB	LEU A 275	14.657	46.253	51.005	1.00 28.58
	MOTA	2142	CG	LEU A 275	14.847	47.735	51.239	1.00 26.78
	ATOM	2143		LEU A 275	16.191	48.183	50.698	1.00 21.90
	ATOM	2144		LEU A 275	13.712	48.478	50.554	1.00 31.48
	MOTA	2145	N	THR A 276	17.062	45.244	53.570	1.00 29.67

	ATOM	2146	CA	THR A	276	17.2	225	45.198	54.996	1.00 30.47
	MOTA	2147	С	THR A	276	17.1	20	46.624	55.597	1.00 34.60
	ATOM	2148	0	THR A		17.7		47.588	55.129	1.00 31.01
	MOTA	2149	CB	THR A		18.5		44.397	55.387	1.00 30.98
5	ATOM	2150	OG1	THR A		18.2		43.030	55.512	1.00 42.01
_	ATOM	2151		THR A		19.1		44.835	56.694	1.00 29.43
	ATOM	2152	N	PHE A		16.2		46.759	56.622	1.00 27.69
									_	
	ATOM		CA	PHE A		16.1		48.034	57.274	1.00 28.92
10	ATOM		C	PHE A		17.1		48.065	58.403	1.00 36.07
10	MOTA		0	PHE A		17.3		47.088	59.131	1.00 34.57
	MO'TA		CB	PHE A		14.7		48.265	57.901	1.00 30.17
	MOTA	2157	CG	PHE A	277	13.7	774	48.458	56.848	1.00 30.72
	ATOM	2158	CD1	PHE A	277	14.0	11	47.966	55.568	1.00 30.73
	ATOM	2159	CD2	PHE A	277	12.5	573	49.114	57.105	1.00 30.61
15	MOTA		CE1	PHE A	277	13.0	172	48.135	54.552	1.00 29.30
	ATOM			PHE A		11.6		49.276	56.101	1.00 32.26
	MOTA		CZ	PHE A		11.8		48.772	54.824	1.00 32.20
	ATOM		N	VAL A		17.8		49.186	58.562	
See and										1.00 32.97
2 Mil.	ATOM		CA	VAL A		18.8		49.338	59.614	1.00 32.66
20	ATOM		C	VAL A		18.6		50.698	60.248	1.00 37.01
(43 ta)(ATOM		0	VAL A		18.2		51.635	59.599	1.00 37.16
je#x	ATOM		CB	VAL A		20.2	246	49.088	59.109	1.00 36.51
144 mm	MOTA	2168		VAL A		20.1	L73	47.967	58.086	1.00 37.40
5 4ks	ATOM	2169	CG2	VAL A	278	20.7	791	50.356	58.444	1.00 34.87
25	-ATOM	2170	N	THR A	279	19.0	066	50.778	61.515	1.00 32.36
	ATOM		CA	THR A		18.9		51.994	62,264	1.00 31.03
-L	ATOM		C	THR A		20.1		52.883	62.035	1.00 37.42
\$	ATOM		ŏ	THR A		21.2		52.397	61.920	1.00 37.42
]=4 ₀	ATOM		CB	THR A		18.8		51.695	63.759	
1.30			OG1							1.00 31.39
	ATOM			THR A		19.1		52.895	64.472	1.00 34.21
	ATOM			THR A		19.9		50.706	64.083	1.00 23.69
in m	ATOM		N	PRO A		19.8		54.187	62.000	1.00 30.07
C)	ATOM		CA	PRO A		20.9		55.132	61.802	1.00 27.00
	ATOM		С	PRO A	280	21.8	323	55.110	63.005	1.00 30.60
35	ATOM	2180	0	PRO A		22.9	951	55.588	62.934	1.00 30.20
	ATOM	2181	CB	PRO A	280	20.2	249	56.497	61.601	1.00 26.23
	ATOM	2182	CG	PRO A	280	18.7	769	56.337	61.889	1.00 28.07
	ATOM	2183	CD	PRO A	280	18.4	199	54.848	61.984	1.00 26.11
	ATOM	2184	N	THR A	281	21.3	348	54.509	64.112	1.00 27.82
40	ATOM		CA	THR A		22.1		54.426	65.302	1.00 27.48
	ATOM		C	THR A		23.3		53.523	65.073	1.00 31.37
	ATOM		Ō	THR A		24.2		53.385	65.944	1.00 31.93
	ATOM		CB	THR A		21.4		54.016	66.601	1.00 21.45
	ATOM			THR A		21.0		52.681	66.524	
45	ATOM			THR A		20.3		54.994		1.00 33.18
-13									66.874	1.00 9.89
	ATOM		N	LEU A		23.3		52.881	63.913	1.00 25.29
	ATOM		CA	LEU A		24.4		51.993	63.586	1.00 24.04
	ATOM		C	LEU A		25.6		52.790	63.049	1.00 34.74
50	ATOM		0	LEU A		26.7		52.279	62.884	1.00 34.84
50			CB	LEU A		24.0	063	51.038	62.464	1.00 22.14
	ATOM		CG	LEU A		23.1	104	49.916	62.819	1.00 26.88
	ATOM			LEU A		23.3	312	48.809	61.791	1.00 27.77
	ATOM	2198	CD2	LEU A	282	23.3	322	49.404	64.249	1.00 21.75
	ATOM	2199	N	LEU A	283	25.4	465	54.063	62.744	1.00 32.05
55	ATOM	2200	CA	LEU A	283	26.5	501	54.903	62.159	1.00 31.43
	ATOM		С	LEU A		27.6		55.324	63.055	1.00 41.94
	ATOM		Ö	LEU A		27.9		56.525	63.196	1.00 49.19
	MOTA		CB	LEU A		25.8		56.117	61.418	1.00 49.19
	ATOM		CG							
60				LEU A		24.		55.661	60.488	1.00 32.94
.00				LEU A		23.9		56.811	59.869	1.00 33.48
	MOTA			LEU A		25.2		54.716	59.409	1.00 28.39
	ATOM		N	ALA A		28.3		54.370	63.638	1.00 33.18
	ATOM		CA	ALA A		29.		54.728	64.532	1.00 30.20
	ATOM	2209	C	ALA A	284	30.6	655	55.492	63.922	1.00 31.97

	ATOM	2210	0	ALA A 284	31.411	56.165	64.642	1.00 31.40
	ATOM	2211	CB	ALA A 284	29.973	53.544	65.336	1.00 29.60
	ATOM	2212	N	GLY A 285	30.801	55.371	62.605	1.00 27.10
_	ATOM	2213	CA	GLY A 285	31.882	56.018	61.867	1.00 29.77
5		2214	С	GLY A 285	33.174	55.194	61.910	1.00 39.25
	ATOM	2215	0	GLY A 285	34.264	55.649	61.544	1.00 41.21
	MOTA	2216	N	ASP A 286	33.022	53.951	62.363	1.00 34.57
	MOTA	2217	CA	ASP A 286	34.144	53.057	62.473	1.00 32.57
10	MOTA	2218	С	ASP A 286	33.805	51.625	62.130	1.00 31.59
10		2219	0	ASP A 286	34.609	50.743	62.325	1.00 29.27
	ATOM	2220	CB	ASP A 286	34.812	53.163	63.860	1.00 34.65
	ATOM	2221	CG	ASP A 286	34.081	52.447	64.945	1.00 41.93
	MOTA	2222		ASP A 286	33.008	51.893	64.765	1.00 45.21
15	MOTA	2223		ASP A 286	34.714	52.492	66.087	1.00 35.67
13		2224	N	LYS A 287	32.590	51.395	61.641	1.00 29.46
	ATOM	2225	CA	LYS A 287	32.199	50.038	61.272	1.00 31.62
use etc.	ATOM	2226	C	LYS A 287	31.976	49.060	62.437	1.00 37.91
	MOTA	2227	O	LYS A 287	31.761	47.879	62.240	1.00 37.91
20	ATOM	2228	CB	LYS A 287	33.215	49.447	60.304	1.00 32.17
45 20		2229	CG	LYS A 287	33.510	50.358	59.119	1.00 51.60
is A.	ATOM	2230	CD	LYS A 287	33.960	49.601	57.877	1.00 50.74
25 min.	ATOM	2231	CE	LYS A 287	35.290	50.105	57.328	1.00 63.80
#2 ## T	ATOM	2232	NZ	LYS A 287	35.167	50.866	56.069	1.00 71.91
25	ATOM	2233 2234	N	SER A 288	32.168	49.575	63.647	1.00 31.58
44 4	ATOM		CA	SER A 288	32.079	48.737	64.810	1.00 27.15
je #	ATOM	2235	C	SER A 288	30.742	48.137	65.142	1.00 36.08
***	ATOM	2236 2237	0	SER A 288	30.676	47.318	66.057	1.00 37.87
ha.	ATOM	2237	CB OG	SER A 288	32.618	49.463	66.005	1.00 16.31
30	ATOM	2239	N	SER A 288	31.659	50.443	66.312	1.00 29.71
n.	ATOM	2240	CA	LEU A 289	29.669	48.529	64.460	1.00 29.34
	ATOM	2241	CA	LEU A 289	28.351	47.979	64.794	1.00 24.70
the mile	ATOM	2242	õ	LEU A 289 LEU A 289	27.792	47.105	63.686	1.00 32.97
	ATOM	2243	СВ	LEU A 289	26.591 27.385	46.766	63.648	1.00 30.35
35	ATOM	2244	CG	LEU A 289	27.954	49.090	65.191	1.00 21.45
	ATOM	2245		LEU A 289	26.881	49.887 50.769	66.347	1.00 22.99
	ATOM	2246		LEU A 289	28.381	48.881	66.950	1.00 20.66
	ATOM	2247	N	SER A 290	28.723	46.753	67.394 62.801	1.00 29.65
	ATOM	2248	CA	SER A 290	28.453	45.941	61.645	1.00 31.21 1.00 29.89
40	MOTA	2249	С	SER A 290	27.861	44.582	62.006	1.00 29.89
	ATOM	2250	0	SER A 290	27.299	43.872	61.153	1.00 30.37
	ATOM	2251	CB	SER A 290	29.704	45.800	60.783	1.00 29.73
	ATOM	2252	OG	SER A 290	30.470	44.725	61.266	1.00 38.77
	ATOM	2253	N	ASN A 291	27.980	44.207	63.282	1.00 26.55
45	ATOM	2254	CA	ASN A 291	27.449	42.909	63.706	1.00 25.78
	ATOM	2255	С	ASN A 291	26.006	42.773	63.355	1.00 30.89
	ATOM	2256		ASN A 291	25.576	41.702	62.975	1.00 29.73
	ATOM	2257		ASN A 291	27.725	42.503	65.157	1.00 28.48
50	ATOM	2258	CG	ASN A 291	26.910	43.313	66.119	1.00 33.33
50	MOTA	2259		ASN A 291	27.065	44.529	66.198	1.00 34.48
	ATOM	2260		ASN A 291	26.001	42.653	66.818	1.00 28.96
	ATOM	2261		VAL A 292	25.277	43.885	63.476	1.00 30.68
	ATOM	2262		VAL A 292	23.865	43.924	63.142	1.00 30.27
55	ATOM	2263		VAL A 292	23.667	43.619	61.669	1.00 32.61
55	ATOM	2264		VAL A 292	22.644	43.082	61.255	1.00 33.31
	ATOM	2265		VAL A 292	23.288	45.289	63.505	1.00 35.13
	ATOM	2266		VAL A 292	21.877	45.486	62.946	1.00 33.48
	ATOM	2267		VAL A 292	23.328	45.478	65.014	1.00 35.02
60	ATOM	2268	N	ILE A 293	24.653	43.975	60.861	1.00 27.92
00	MOTA	2269		ILE A 293	24.527	43.685	59.461	1.00 28.71
	ATOM	2270		ILE A 293	24.658	42.159	59.296	1.00 35.03
	ATOM	2271		ILE A 293	23.860	41.475	58.624	1.00 38.34
	ATOM	2272		ILE A 293	25.554	44.438	58.606	1.00 33.84
	ATOM	2273	CGI	ILE A 293	25.608	45.952	58.898	1.00 34.55

	MOTA	2274	CG2	ILE A 29	3	25.305	44.186	57.121	1.00 36.50
	ATOM	2275		ILE A 29		24.265	46.680	58.808	1.00 30.49
		2276		ALA A 29		25.668	41.584	59.934	1.00 23.76
	ATOM								
_	ATOM	2277		ALA A 29		25.836	40.138	59.809	1.00 19.95
5	MOTA	2278	С	ALA A 29	4	24.559	39.409	60.165	1.00 27.33
	MOTA	2279	0	ALA A 29	4	24.183	38.422	59.505	1.00 25.48
	ATOM	2280		ALA A 29		26.984	39.644	60.688	1.00 19.24
				HIS A 29		23.917	39.934	61.244	1.00 27.63
	ATOM	2281							
4.0	ATOM	2282		HIS A 29		22.666	39.414	61.797	1.00 26.83
10	ATOM	2283	С	HIS A 29	5	21.611	39.383	60.734	1.00 28.61
	MOTA	2284	0	HIS A 29	5	21.169	38.301	60.348	1.00 25.72
	ATOM	2285		HIS A 29		22.148	40.175	63.028	1.00 27.98
				HIS A 29					
	MOTA	2286				20.937	39.534	63.657	1.00 31.62
	MOTA	2287	ND1	HIS A 29	5	21.047	38.675	64.763	1.00 32.66
15	ATOM	2288	CD2	HIS A 29	5	19.602	39.643	63.338	1.00 30.92
	ATOM	2289	CE1	HIS A 29	5	19.802	38.298	65.088	1.00 30.14
	ATOM	2290		HIS A 29		18.916	38.860	64.254	1.00 30.24
3									
	MOTA	2291	N	GLU A 29		21.257	40.590	60.251	1.00 27.23
349	MOTA	2292	CA	GLU A 29	6	20.266	40.749	59.195	1.00 25.98
20	ATOM	2293	С	GLU A 29	6	20.533	39.790	58.056	1.00 32.73
145 #	ATOM	2294	0	GLU A 29		19.628	39.081	57.561	1.00 31.88
h-Ac		2295	СВ	GLU A 29		20.046	42.203	58.728	
n Esta	ATOM								1.00 24.55
· · · · · · · · · · · · · · · · · · ·	MOTA	2296	CG	GLU A 29		19.892	43.148	59.936	1.00 23.16
25	MOTA	2297	CD	GLU A 29		18.939	42.632	60.991	1.00 53.50
25	MOTA	2298	OE1	GLU A 29	16	17.964	41.956	60.700	1.00 23.99
\$4 K	ATOM	2299		GLU A 29		19.237	43.006	62.233	1.00 32.77
- i									
*	ATOM	2300	N	ILE A 29		21.803	39.745	57.675	1.00 25.37
	MOTA	2301	CA	ILE A 29		22.195	38.870	56.599	1.00 22.64
##.	MOTA	2302	С	ILE A 29	7	21.812	37.445	56.859	1.00 27.47
30	MOTA	2303	0	ILE A 29	7	21.175	36.799	56.048	1.00 26.25
	MOTA	2304	СВ	ILE A 29		23.672	38.963	56.302	1.00 24.19
6 22									
2 m	MOTA	2305	CG1			23.920	40.140	55.355	1.00 25.28
7%	ATOM	_ 2306	CG2	ILE A 29	97	24.079	37.686	55.626	1.00 20.77
\$4.40°	ATOM	2307	CD1	ILE A 29	37	25.325	40.705	55.435	1.00 16.26
35	ATOM	2308	N	SER A 29	8	22.226	36.947	58.012	1.00 28.23
	MOTA	2309	CA	SER A 29		21.939	35.569	58.377	1.00 25.04
	MOTA	2310	С	SER A 29		20.467	35.235	58.298	1.00 26.21
	ATOM	2311	0	SER A 29		20.118	34.097	58.000	1.00 26.30
	ATOM	2312	CB	SER A 29	98	22.520	35.209	59.714	1.00 27.82
40	ATOM	2313	OG	SER A 29	8	23.890	35.552	59.714	1.00 35.98
*	ATOM	2314	N	HIS A 29		19.599	36.230	58.562	1.00 22.17
	MOTA	2315	CA	HIS A 29		18.205	36.092	58.719	1.00 22.77
	MOTA	2316	C	HIS A 29		17.614	35.710	57.387	1.00 29.10
	MOTA	2317	0	HIS A 29	9	16.553	35.162	57.290	1.00 31.50
45	ATOM	2318	CB	HIS A 29	9	17.662	37.432	59.200	1.00 24.67
	ATOM	2319	CG	HIS A 29	19	17.053	37.338	60.602	1.00 29.10
	ATOM	2320		HIS A 29					
						16.190	36.368	60.975	1.00 30.70
	MOTA	2321		HIS A 29		17.196	38.233	61.667	1.00 32.39
	MOTA	2322		HIS A 29		15.811	36.675	62.233	1.00 30.41
50	MOTA	2323	NE2	HIS A 29	99	16.397	37.783	62.674	1.00 31.74
	ATOM	2324	N	SER A 30		18.356	36.048	56.315	1.00 23.31
		2325	CA						
	ATOM			SER A 30		17.942	35.581	55.010	1.00 24.24
	ATOM	2326	С	SER A 30		17.879	34.050	54.977	1.00 34.13
	ATOM	2327	0	SER A 30	00	17.075	33.463	54.305	1.00 33.28
- 55	MOTA	2328	CB	SER A 30		18.941	36.092	53.965	1.00 27.31
	MOTA	2329	OG	SER A 30		18.947	37.519	53.962	
									1.00 49.96
	MOTA	2330	N	TRP A 3		18.773	33.411	55.752	1.00 33.09
	ATOM	2331	CA	TRP A 30	01	18.702	31.969	55.829	1.00 31.84
	ATOM	2332	С	TRP A 30		17.740	31.511	56.895	1.00 32.15
60	ATOM	2333	ŏ	TRP A 3		16.764	30.876	56.620	1.00 27.05
00									
	MOTA	2334	CB	TRP A 3		20.095	31.429	56.082	1.00 30.16
	ATOM	2335	CG	TRP A 3		20.791	31.421	54.801	1.00 32.02
	MOTA	2336		TRP A 3		20.787	30.393	53.859	1.00 35.05
	ATOM	2337		TRP A 3		21.496	32.520	54.202	1.00 30.84
					_				

		MOTA	2338	NEI	TRP A	301	21.415	30.732	52.722	1.00 33.29
		ATOM	2339		TRP A		21.886	32.112	52.921	1.00 33.44
		ATOM	2340		TRP A		21.811	33.790	54.631	1.00 32.65
		ATOM	2341		TRP A		22.577	32.970	52.108	1.00 32.21
5	,	ATOM	2342		TRP A		22.503	34.652	53.812	1.00 36.10
	•	ATOM	2343		TRP A		22.888	34.239	52.544	1.00 36.83
		MOTA	2344		THR A		18.042	31.864	58.146	1.00 31.77
		ATOM	2345		THR A		17.125	31.488	59.215	1.00 33.55
		ATOM	2346		THR A		16.276	32.690	59.695	1.00 36.35
10	•	ATOM	2347		THR A		16.759	33.590	60.330	1.00 36.56
.10		ATOM	2348		THR A		17.963	30.920	60.366	1.00 31.04
		ATOM	2349		THR A		19.047	31.807	60.639	1.00 38.50
		ATOM	2350		THR A		18.544	29.555	59.967	1.00 30.30
		MOTA	2351	N	GLY A		15.053	32.418	59.250	1.00 25.28
15	ξ	ATOM	2352	CA	GLY A		13.908	33.236	59.483	1.00 23.20
1.		ATOM	2353	C	GLY A		13.202	33.382	58.163	1.00 21.39
			2354	o	GLY A		12.040	33.040	57.994	
		ATOM	2355		ASN A		13.936	33.891	57.195	1.00 26.18
# F.		ATOM	2356		ASN A					1.00 28.05
	1	ATOM			ASN A		13.363	34.101	55.875	1.00 28.17
1 20	,	ATOM	2357				13.141	32.839	55.056	1.00 28.99
W.		MOTA	2358	0	ASN A		12.118	32.715	54.415	1.00 24.87
in a sing		MOTA	2359		ASN A		14.091	35.176	55.047	1.00 23.55
## ## ## ## ## ## ## ## ## ## ## ## ##		ATOM	2360	CG	ASN A		14.133	36.499	55.757	1.00 37.80
1 2	_	ATOM	2361		ASN A		13.630	36.613	56.892	1.00 20.66
2:	•	ATOM	2362		ASN A		14.752	37.488	55.093	1.00 24.17
124 · (1		ATOM	2363	N	LEU A		14.110	31.919	55.055	1.00 27.24
jak,		ATOM	2364	CA	LEU A		13.987	30.677	54.306	1.00 27.34
畢		MOTA	2365	С	LEU A		13.218	29.665	55.121	1.00 31.29
L.		MOTA	2366	0	LEU A		12.235	29.051	54.678	1.00 29.23
74 30	U ,	ATOM	2367	CB	LEU A		15.371	30.119	53.967	1.00 27.62
		ATOM	2368	CG	LEU A		15.805	30.593	52.603	1.00 32.23
#####################################		ATOM	2369		LEU A		17.289	30.293	52.412	1.00 28.91
15 11		MOTA	2370		LEU A		14.951	29.887	51.549	1.00 41.51
-	_	MOTA	2371	N	VAL A		13.711	29.528	56.347	1.00 27.75
L. 3.	5	MOTA	2372	CA	VAL A		13.134	28.652	57.327	1.00 29.99
		ATOM	2373	С	VAL A		12.578	29.527	58.403	1.00 31.78
•		ATOM	2374	0	VAL A		13.306	30.217	59.110	1.00 28.32
		ATOM	2375	CB	VAL A		14.092	27.593	57.827	1.00 37.24
	_	ATOM	2376		VAL A		15.479	28.180	57.969	1.00 38.36
4	U	ATOM	2377	CG2	VAL A		13.602	27.107	59.164	1.00 37.56
		ATOM	2378	N	THR A		11.259	29.517	58.440	1.00 29.40
		MOTA	2379	CA	THR A		10.499	30.358	59.320	1.00 28.14
		MOTA	2380	С	THR A		9.729	29.712	60.446	1.00 34.06
	_	ATOM	2381	0	THR A		9.029	28.706	60.277	1.00 36.72
4	3	MOTA	2382	CB	THR A		9.474	31.115	58.460	1.00 23.03
		ATOM	2383		THR A		10.124	31.811	57.422	1.00 28.56
		ATOM	2384		THR A		8.665	32.068	59.336	1.00 12.55
		ATOM	2385	N	ASN A		9.802	30.347	61.608	1.00 29.29
_	^	MOTA	2386	CA	ASN A		9.042	29.862	62.724	1.00 27.82
)	0	ATOM	2387	С	ASN A		7.576	29.716	62.234	1.00 31.42
		ATOM	2388	0	ASN A		7.072	30.535	61.450	1.00 32.96
		ATOM	2389	CB	ASN A		9.194	30.790	63.972	1.00 23.57
		ATOM	2390	ÇG	ASN A		8.935	32.298	63.745	1.00 30.38
_	_	ATOM	2391		ASN A		9.505	33.190	64.400	1.00 23.70
5	5	ATOM	2392	ND2	ASN A		8.056	32.608	62.818	1.00 41.34
		ATOM	2393	N	LYS A		6.890	28.658	62.640	1.00 24.10
		ATOM	2394	CA	LYS A		5.502	28.433	62.230	1.00 23.40
		ATOM	2395	С	LYS A		4.514	29,380	62.964	1.00 28.17
_	. ~	ATOM	2396	0	LYS A		3.430	29.756	62.474	1.00 22.88
. 6	0	ATOM	2397	CB	LYS A		5.151	26.975	62.459	1.00 24.26
		MOTA	2398	CG	LYS A		4.036	26.478	61.555	1.00 28.57
		MOTA	2399	CD	LYS A		3.543	25.075	61.924	1.00 38.25
		MOTA	2400	CE	LYS A		3.475	24.112	60.739	1.00 78.39
		MOTA	2401	NZ	LYS A	309	4.389	22.953	60.849	1.00 98.22

	ATOM	2402	N	THR A 31	.0	4.917	29.744	64.179	1.00	23.46
	ATOM	2403	CA	THR A 31		4.179	30.616	65.037		22.98
	MOTA	2404	С	THR A 31	.0	5.142	31.336	65.922	1.00	31.43
	MOTA	2405	0	THR A 31	.0	6.223	30.836	66.230	1.00	31.51
5	ATOM	2406	CB	THR A 31	.0	3.104	29.917	65.871	1.00	34.01
	ATOM	2407	OG1	THR A 31	10	3.684	29.148	66.945	1.00	27.97
	MOTA	2408	CG2	THR A 31	.0	2.174	29.114	64.956	1.00	24.58
	ATOM	2409	N	TRP A 31	.1	4.733	32.527	66.299	1.00	29.82
	MOTA	2410	CA	TRP A 31	11	5.559	33.371	67.120	1.00	30.49
10	MOTA	2411	С	TRP A 31	11	6.044	32.692	68.381	1.00	26.99
	MOTA	2412	0	TRP A 31	1	7.015	33.101	68.971	1.00	25.15
	ATOM	2413	CB	TRP A 31	L1	4.933	34.768	67.320	1.00	30.34
	ATOM	2414	CG	TRP A 31	11	4.706	35.412	66.001	1.00	30.63
	ATOM	2415	CD1	TRP A 31	11	3.514	35.785	65.490	1.00	32.07
15	MOTA	2416	CD2	TRP A 31	11	5.705	35.723	65.008	1.00	31.31
	MOTA	2417	NE1	TRP A 31	L1	3.703	36.335	64.250	1.00	29.97
	MOTA	2418	CE2	TRP A 31	L1	5.033	36.317	63.931	1.00	32.88
24 FB.	ATOM	2419	CE3	TRP A 3	L 1	7.099	35.586	64.943	1.00	31.44
	MOTA	2420	CZ2	TRP A 31	11	5.721	36.771	62.804	1.00	31.56
- 20	ATOM	2421	CZ3	TRP A 3	11	7 .7 79	36.059	63.848	1.00	30.39
ui.	MOTA	2422	CH2	TRP A 3	11	7.089	36.639	62.789	1.00	30.58
	ATOM	2423	N	ASP A 3	12	5.366	31.632	68.770	1.00	27.36
सर्वे सार इसर	ATOM	2424	CA	ASP A 3	12	5.757	30.868	69.950	1.00	27.38
= 200	ATOM	2425	С	ASP A 3	L2	7.149	30.213	69.757	1.00	31.25
25	ATOM	2426	0	ASP A 3	12	7.826	29.802	70.718	1.00	27.07
## X	ATOM	2427	CB	ASP A 3	12	4.697	29.750	70.217	1.00	25.96
}=&.	MOTA	2428	CG	ASP A 3	12	3.432	30.230	70.872	1.00	27.42
#	ATOM	2429	OD1	ASP A 3	12	3.197	31.396	71.102	1.00	28.97
	ATOM	2430	OD2	ASP A 3		2.623	29.265	71.208	1.00	29.33
-30	ATOM	2431	N	HIS A 3		7.562	30.089	68.487	1.00	25.04
F.	ATOM	2432	CA	HIS A 3		8.820	29.454	68.164	1.00	23.48
	ATOM	2433	С	HIS A 3		9.864	30.452	67.737		25.38
55 M	MOTA	2434	0	HIS A 3		10.929	30.139	67.214		29.97
	MOTA	2435	CB	HIS A 3		8.588	28.245	67.209		25.00
-35	MOTA	2436	CG	HIS A 3		7.641	27.230	67.837		29.77
	ATOM	2437		HIS A 3		8.087	26.183	68.635	1.00	31.37
	MOTA	2438		HIS A 3		6.279	27.152	67.808		31.31
	ATOM	2439		HIS A 3		7.015	25.509	69.039		28.91
40	MOTA	2440		HIS A 3		5.913	26.066	68.559		29.40
40	MOTA	2441	N	PHE A 3		9.521	31.682	68.005		17.43
	ATOM	2442	CA	PHE A 3		10.345	32.810	67.701		17.16
	ATOM	2443	C	PHE A 3		11.852	32.523	67.812		26.01
	ATOM	2444	0	PHE A 3		12.669	32.922	66.963		30.40
45	ATOM	2445	CB	PHE A 3		9.908	34.056	68.517		18.63
43	MOTA	2446				10.592	35.351	68.113		20.10
	MOTA MOTA	2447 2448		PHE A 3		10.712 11.129	35.697 36.214	66.768		21.80
	ATOM	2449		PHE A 3				69.070		22.60
	ATOM	2450		PHE A 3		11.337 11.750	36.890 37.416	66.400 68.716		24.74 27.24
50	ATOM	2451	CZ	PHE A 3		11.750	37.756	67.368		24.97
20	ATOM	2452	N	TRP A 3		12.235	31.828	68.861		19.66
	ATOM	2453	CA	TRP A 3		13.639	31.541	69.068		17.87
	ATOM	2454	C	TRP A 3		14.292	30.775	67.953		28.55
	ATOM	2455	Õ	TRP A 3		15.518	30.769	67.830		29.23
55	ATOM	2456	СВ	TRP A 3		13.860	30.842	70.362		16.03
	ATOM	2457	CG	TRP A 3		13.613	29.408	70.362		19.64
	ATOM	2458		TRP A 3		12.428	28.787	70.101		22.39
	MOTA	2459		TRP A 3		14.599	28.430	69.876		21.70
	MOTA	2460		TRP A 3		12.597	27.457	70.033		24.22
60	ATOM	2461		TRP A 3		13.934	27.205	69.801		27.96
-	ATOM	2462		TRP A 3		15.976	28.481	69.681		22.89
	ATOM	2463		TRP A 3		14.631	26.018	69.547		27.76
	ATOM	2464		TRP A 3		16.651	27.321	69.421		23.16
	ATOM	2465		TRP A 3		15.991	26.108	69.341		23.94
			_							

	ATOM	2466	N	LEU A	316	13.488	30.114	67.144	1.00 26.33
	ATOM	2467	CA	LEU A		14.092	29.400	66.067	1.00 25.44
	ATOM	2468	С	LEU A	316	14.666	30.443	65.129	1.00 33.21
	ATOM	2469	0	LEU A	316	15.737	30.252	64.530	1.00 37.80
5	ATOM	2470	CB	LEU A	316	13.050	28.567	65.311	1.00 24.82
	ATOM	2471	CG	LEU A		12.663	27.242	65.956	1.00 27.62
	MOTA	2472	CD1	LEU A		11.574	26.552	65.106	1.00 22.30
	MOTA	2473	CD2	LEU A	316	13.897	26.344	66.097	1.00 27.03
	MOTA	2474	N	ASN A	317	13.931	31.555	64.997	1.00 20.55
10	MOTA	2475	CA	ASN A	317	14.354	32.624	64.115	1.00 19.34
10		2476	C	ASN A					
	MOTA					15.603	33.333	64.531	1.00 30.38
	MOTA	2477	0	ASN A		16.553		63.766	1.00 32.04
	ATOM	2478	CB	ASN A	317	13.273	33.682	63.838	1.00 14.82
	MOTA	2479	CG	ASN A	317	12.330	33.177	62.793	1.00 31.14
15	ATOM	2480		ASN A		12.151	31.966	62.657	1.00 38.42
10									
	ATOM	2481		ASN A		11.724	34.074	62.049	1.00 17.34
	ATOM	2482	N	GLU A		15.562	33.870	65.750	1.00 26.15
	ATOM	2483	CA	GLU A	318	16.624	34.648	66.358	1.00 20.23
57 PL	ATOM	2484	С	GLU A	318	17.860	33.884	66.816	1.00 23.53
20	ATOM	2485	Ö	GLU A		19.006		66.554	1.00 26.34
32 22									
43	ATOM	2486	CB	GLU A		15.998		67.456	1.00 19.11
	ATOM	2487	CG	GLU A		14.999	36.480	66.800	1.00 24.06
1-1.	ATOM	2488	CD	GLU A	318	15.615	37.391	65.758	1.00 40.32
16 mrs	ATOM	2489	OE1	GLU A		16.833		65.612	1.00 21.24
25		2490	OE2	GLU A		14.703			
# 14th	ATOM							65.062	1.00 24.23
	ATOM	2491	N	GLY A		17.621		67.494	1.00 17.17
1-2	MOTA	2492	CA	GLY A		18.681	31.955	68.016	1.00 15.31
*	MOTA	2493	С	GLY A	319	19.673	31.601	66.953	1.00 24.07
	MOTA	2494	0	GLY A	319	20.860	31.897	67.080	1.00 28.47
30	ATOM	2495	N	HIS A		19.165		65.907	1.00 20.24
13	ATOM	2496	CA	HIS A		19.977		64.790	
									1.00 20.13
र्वे करोते. अस्य देवा	MOTA	2497	C	HIS A		20.678		64.142	1.00 24.97
	ATOM	2498	0	HIS A		21.855	31.700	63.739	1.00 23.54
E 25	ATOM	-2499	CB	HIS P	A 320	19.143	29.737	63.791	1.00 20.57
35	ATOM	2500	CG	HIS A	320	18.662	28.426	64.349	1.00 22.57
Handar .	ATOM	2501	ND1	HIS A	320	17.471		65.058	1.00 22.98
	ATOM	2502		HIS A		19.217		64.286	1.00 19.52
		2503							
	ATOM			HIS A		17.336		65.385	1.00 19.18
40	ATOM	2504		HIS A		18.368		64.952	1.00 18.12
40	ATOM	2505	N	THR A		19.958	32.875	64.053	1.00 21.61
	MOTA	2506	CA	THR A	321	20.543	34.056	63.478	1.00 22.16
	ATOM	2507	С	THR A	321	21.697	34.552	64.342	1.00 27.47
	ATOM	2508	0	THR A		22.789		63.836	1.00 26.64
	ATOM	2509	CB	THR A		19.470		63.113	1.00 27.88
15									
45	MOTA	2510		THR A		18.403		62.523	1.00 27.92
	ATOM	2511		THR A		19.999		62.087	1.00 18.05
	ATOM	2512	N	VAL A	322	21.496	34.634	65.659	1.00 21.90
	ATOM	2513	CA	VAL A	322	22.610	35.054	66.470	1.00 19.44
	ATOM	2514	С	VAL A		23.762		66.285	1.00 24.43
50	MOTA	2515	ō	VAL A					
50						24.926		66.188	1.00 21.48
	MOTA	2516	CB	VAL A		22.218		67.928	1.00 20.92
	ATOM	2517	CG1	VAL A	A 322	23.406	35.644	68.772	1.00 18.37
	MOTA	2518	CG2	VAL A	322	21.093	36.200	68.048	1.00 20.01
	ATOM	2519	N	TYR A	323	23.427		66.197	1.00 27.08
55	ATOM	2520	CA	TYR A		24.446		66.013	1.00 26.26
	MOTA	2521	C	TYR A					
						25.222		64.728	1.00 28.26
	ATOM	2522	0	TYR A		26.431		64.643	1.00 27.51
	MOTA	2523	CB	TYR A		23.804	30.407	66.020	1.00 25.74
	MOTA	2524	CG	TYR A	A 323	24.867	29.341	65.987	1.00 26.66
60	ATOM	2525	CD1	TYR A		25.539		67.150	1.00 29.09
~	ATOM	2526		TYR A		25.199		64.789	1.00 24.52
		2527							
	ATOM			TYR A		26.530		67.157	1.00 22.56
	ATOM	2528		TYR A		26.178		64.770	1.00 25.31
	MOTA	2529	CZ	TYR A	A 323	26.846	27.370	65.944	1.00 29.19

	ATOM	2530	OH	TYR A 323	27.823	26.434	65.895	1.00 27.51
	ATOM	2531	N	LEU A 324	24.497	32.408	63.702	1.00 24.82
	ATOM	2532	CA	LEU A 324	25.135	32.638	62.439	1.00 26.04
-	MOTA	2533	C	LEU A 324	25.832	33.952	62.417	1.00 30.92
5	ATOM	2534	0	LEU A 324	26.903	34.045	61.851	1.00 33.76
	ATOM	2535	CB	LEU A 324	24.176	32.537	61.235	1.00 26.21
	ATOM	2536	CG	LEU A 324	23.916	31.112	60.778	1.00 28.46
	ATOM	2537		LEU A 324 LEU A 324	22.752 25.169	31.109 30.508	59.791 60.151	1.00 28.95
10	ATOM	2538 2539	N	GLU A 325	25.234	34.976	63.033	1.00 26.54 1.00 27.04
10	ATOM	2540	CA	GLU A 325	25.870	36.303	63.064	1.00 27.04
	ATOM	2541	C	GLU A 325	27.282	36.210	63.624	1.00 28.76
	ATOM	2542	Õ	GLU A 325	28.250	36.722	63.024	1.00 26.70
	ATOM	2543	CB	GLU A 325	25.016	37.365	63.759	1.00 20.24
15	ATOM	2544	CG	GLU A 325	25.827	38.411	64.524	1.00 41.55
10	MOTA	2545	CD	GLU A 325	25.035	39.040	65.646	1.00 72.11
	ATOM	2546		GLU A 325	23.866	38.764	65.862	1.00 41.88
	ATOM	2547	OE2	GLU A 325	25.719	39.922	66.350	1.00 67.15
27 PR.	ATOM	2548	N	ARG A 326	27.349	35.479	64.755	1.00 27.84
20	ATOM	2549	CA	ARG A 326	28.551	35.213	65.511	1.00 28.10
44	ATOM	2550	C	ARG A 326	29.604	34.457	64.771	1.00 30.90
43	MOTA	2551	0	ARG A 326	30.763	34.747	64.976	1.00 33.93
j=h,	MOTA	2552	CB	ARG A 326	28.334	34.761	66.947	1.00 31.52
wint.	ATOM	2553	CG	ARG A 326	27.645	35.864	67.726	1.00 22.20
25	ATOM	2554	CD	ARG A 326	27.462	35.572	69.203	1.00 28.71
LT.	ATOM	2555	NE	ARG A 326	26.727	36.673	69.830	1.00 23.82
je i.	ATOM	2556	CZ	ARG A 326	25.805	36.556	70.780	1.00 26.09
	MOTA	2557		ARG A 326	25.443	35.388	71.305	1.00 23.16
#	ATOM	2558	NH2	ARG A 326	25.220	37.655	71.222	1.00 24.77
130 []	ATOM	2559	N	HIS A 327	29.221	33.511	63.918	1.00 29.85
	ATOM	2560	CA	HIS A 327	30.207	32.777	63.120	1.00 30.52
	ATOM	2561	С	HIS A 327	30.778	33.738	62.085	1.00 35.50
13.11	ATOM	2562	0	HIS A 327	31.966	33.777	61.822	1.00 36.74
35	ATOM	2563	CB	HIS A 327	29.591	31.555	62.407	1.00 31.59
33	ATOM	2564	CG	HIS A 327	29.764	30.259	63.176	1.00 34.51
H.	ATOM	2565		HIS A 327 HIS A 327	30.963	29.913	63.788	1.00 36.17
	ATOM ATOM	2566 2567 ·		HIS A 327	28.875 30.778	29.263 28.740	63.432 64.384	1.00 35.58 1.00 35.27
	ATOM	2568	NE2		29.532	28.322	64.191	1.00 35.27
40	ATOM	2569	N	ILE A 328	29.902	34.549	61.511	1.00 33.30
	ATOM	2570	CA	ILE A 328	30.328	35.517	60.528	1.00 31.66
	ATOM	2571	C	ILE A 328	31.416	36.407	61.086	1.00 40.12
	ATOM	2572	ō	ILE A 328	32.451	36.615	60.465	1.00 40.81
	ATOM	2573	СВ	ILE A 328	29.175	36.379	59.998	1.00 32.94
45	ATOM	2574	CG1	ILE A 328	28.220	35.570	59.114	1.00 29.53
	ATOM	2575	CG2	ILE A 328	29.694	37.591	59.201	1.00 30.91
	MOTA	2576		ILE A 328	27.119	36.463	58.535	1.00 32.98
	MOTA	2577	N	CYS A 329	31.179	36.948	62.266	1.00 37.88
	ATOM	2578	CA	CYS A 329	32.170	37.810	62.851	1.00 39.54
50	ATOM	2579	С	CYS A 329	33.475	37.092	63.157	1.00 40.19
	ATOM	2580	0	CYS A 329	34.567	37.642	62.971	1.00 38.44
	MOTA	2581	CB	CYS A 329	31.607	38.509	64.083	1.00 42.61
	MOTA	2582	SG	CYS A 329	30.241	39.595	63.619	1.00 48.14
ے ہے	MOTA	2583	N	GLY A 330	33.332	35.852	63 .6 32	1.00 34.74
55	ATOM	2584	CA	GLY A 330	34.471	35.030	63.980	1.00 35.20
	ATOM	2585	C	GLY A 330	35.359	34.854	62.778	1.00 43.66
	ATOM	2586	0	GLY A 330	36.581	34.857	62.891	1.00 46.79
	ATOM	2587	N	ARG A 331	34.709	34.725	61.622	1.00 34.99
60	ATOM	2588	CA	ARG A 331	35.416	34.562	60.392	1.00 33.19
OU	MOTA	2589	C	ARG A 331	36.086	35.863	60.017	1.00 40.63
	MOTA	2590	O	ARG A 331	37.238	35.914	59.586	1.00 44.40
	ATOM	2591	CB	ARG A 331	34.494	34.101	59.269	1.00 31.29
	MOTA	2592	CG	ARG A 331	33.987	32.685	59.450	1.00 47.66
	MOTA	2593	CD	ARG A 331	34.812	31.722	58.622	1.00 70.36

	MOTA	2594	NE	ARG A		34.461	31.851	57.221	1.00 80.25
	ATOM	2595	CZ	ARG A	331	33.615	31.023	56.628	1.00100.00
	MOTA	2596	NH1	ARG A	331	33.055	29.999	57.279	1.00 79.12
	ATOM	2597	NH2	ARG A	331	33.334	31.216	55.341	1.00 89.33
5	ATOM	2598	N	LEU A		35.342	36.926	60.172	1.00 32.14
	ATOM	2599	CA	LEU A		35.885	38.198	59.820	1.00 30.02
	ATOM	2600	C	LEU A		37.013	38.612		
								60.761	1.00 40.33
	MOTA	2601	0	LEU A		38.084	38.972	60.286	1.00 40.10
10	MOTA	2602	CB	LEU A		34.772	39.262	59.822	1.00 28.20
10	ATOM	2603	CG	LEU A		34.451	39.896	58.469	1.00 28.82
	MOTA	2604		LEU A		35.007	39,063	57.341	1.00 23.73
	MOTA	2605	CD2	LEU A	332	32.947	40.114	58.306	1.00 29.76
	ATOM	2606	N	PHE A		36.744	38.557	62.091	1.00 37.69
	ATOM	2607	CA	PHE A		37.657	38.997	63.143	1.00 34.12
15	ATOM	2608	C	PHE A		38.251	37.956	64.035	1.00 37.12
13	ATOM	2609	Ö	PHE A					
						39.015	38.293	64.925	1.00 41.67
	ATOM	2610	CB	PHE A		36.970	40.058	64.024	1.00 35.62
	ATOM	2611	CG	PHE A		36.209	41.003	63.138	1.00 39.09
23	MOTA	2612	CD1	PHE A	333	36.887	41.923	62.332	1.00 43.22
20	ATOM	2613	CD2	PHE A	333	34.818	40.941	63.045	1.00 42.78
**************************************	MOTA	2614	CE1	PHE A	333	36.205	42.781	61.464	1.00 44.14
40	MOTA	2615		PHE A		34.123	41.806	62.194	1.00 46.56
- A	ATOM	2616	CZ	PHE A		34.814	42.716	61.389	1.00 43.20
g PAN vertical	ATOM	2617	N	GLY A		37.908	36.706		
25								63.865	1.00 34.36
# 2J	ATOM	2618	CA	GLY A		38.507	35.705	64.763	1.00 32.89
UT .	MOTA	2619	C	GLY A		37.582	34.985	65.767	1.00 32.67
-	ATOM	2620	0	GLY A		36.641	35.540	66.340	1.00 33.48
	ATOM	2621	N	GLU A	335	37.908	33.726	66.003	1.00 23.52
	MOTA	2622	CA	GLU A	335	37.196	32.875	66.931	1.00 18.13
30	MOTA	2623	С	GLU A	335	37.278	33.384	68.346	1.00 29.15
	ATOM	2624	0	GLU A	335	36.357	33.124	69.112	1.00 34.14
	ATOM	2625	CB	GLU A		37.782	31.488	66.929	1.00 17.35
	ATOM	2626	CG	GLU A		37.041	30.591	67.929	1.00 32.97
ing self	ATOM	2627	CD	GLU A		35.642	30.305	67.473	1.00 32.97
35	ATOM	2628	OE1						
1 33				GLU A		35.093	30.944	66.588	1.00 39.31
	ATOM	2629	OE2	GLU A		35.080	29.317	68.132	1.00 32.80
	ATOM	2630	N	LYS A		38.370	34.077	68.706	1.00 24.53
	MOTA	2631	ÇA	LYS A		38.468	34.609	70.061	1.00 25.38
4.0	ATOM	2632	С	LYS A		37.445	35.726	70.169	1.00 35.32
40	ATOM	2633	0	LYS A	336	36.908	36.004	71.233	1.00 38.14
	MOTA	2634	CB	LYS A	336	39.820	35.199	70.421	1.00 25.45
	ATOM	2635	CG	LYS A	336	40.871	34.188	70.825	1.00 25.43
	ATOM	2636	CD	LYS A		42.207	34.846	71.189	1.00 47.10
	ATOM	2637	CE	LYS A	336	43.325	34.600	70.172	1.00 68.74
45	ATOM	2638	NZ	LYS A		44.566	34.072	70.767	1.00 77.62
	ATOM	2639	N	PHE A		37.174	36.364	69.029	1.00 77.02
	ATOM	2640	CA	PHE A					
						36.186	37.442	68.967	1.00 29.34
	ATOM	2641	C	PHE A		34.783	36.869	69.083	1.00 31.73
50	MOTA	2642	0	PHE A		33.908	37.424	69.742	1.00 35.53
50	ATOM	2643	CB	PHE A		36.304	38.336	67.709	1.00 30.04
	ATOM	2644	CG	PHE A		35.435	39.589	67.747	1.00 35.16
	ATOM	2645	CD1	PHE A	337	35.468	40.459	68.843	1.00 43.88
	ATOM	2646	CD2	PHE A	337	34.550	39.893	66.709	1.00 40.16
	ATOM	2647	CE1	PHE A	337	34.688	41.617	68.913	1.00 46.53
55	ATOM	2648		PHE A		33.753	41.040	66.760	1.00 45.62
	ATOM	2649	CZ	PHE A		33.830	41.908	67.852	1.00 45.57
	ATOM	2650	N	ARG A					
						34.566	35.733	68.452	1.00 25.52
	ATOM	2651	CA	ARG A		33.266	35.119	68.508	1.00 25.23
<i>(</i>	ATOM	2652	C	ARG A		32.944	34.759	69.922	1.00 29.77
60	MOTA	2653	0	ARG A		31.854	35.025	70.415	1.00 31.81
	ATOM	2654	CB	ARG A		33.186	33.920	67.606	1.00 24.04
	MOTA	2655	CG	ARG A		31.839	33.228	67.623	1.00 21.31
	ATOM	2656	CD	ARG A		31.807	32.086	66.599	1.00 30.62
	ATOM	2657	NE	ARG A		32.518	30.892	67.040	1.00 29.87
								0	

	MOTA	2658	CZ	ARG A	338	31.919	29.781	67.466	1.00	26.37
				ARG A						20.26
	ATOM	2659				30.616	29.687	67.518		
	ATOM	2660		ARG A		32.632	28.737	67.864		18.57
_	ATOM	2661	N	HIS A		33.934	34.190	70.577		25.88
5	ATOM	2662	CA	HIS A	339	33.813	33.797	71.982	1.00	25.59
	ATOM	2663	С	HIS A	339	33.455	34.972	72.892	1.00	27.61
	MOTA	2664	0	HIS A	339	32.615	34.912	73.793	1.00	25.27
	ATOM	2665	CB	HIS A		35.065	33.045	72.462		25.06
	ATOM	2666	CG	HIS A		34.923	31.587	72.155		28.13
10				HIS A						
10	ATOM	2667				35.049	30.612	73.127		30.52
	ATOM	2668		HIS A		34.586	30.970	70.981		30.89
	MOTA	2669		HIS A		34.843	29.442	72.535	1.00	30.89
	MOTA	2670	NE2	HIS A		34.546	29.616	71.245	1.00	31.36
	MOTA	2671	N	PHE A	340	34.103	36.065	72.608	1.00	24.54
15	MOTA	2672	CA	PHE A	340	33.892	37.278	73.334	1.00	25.36
	ATOM	2673	С	PHE A		32.452	37.762	73.216		32.47
	ATOM	2674	Ō	PHE A		31.822	38.222	74.190		32.78
		2675	CB	PHE A		34.876	38.309	72.801		
	ATOM									26.03
	ATOM	2676	CG	PHE A		34.654	39.671	73.346		26.47
20	MOTA	2677		PHE A		35.238	40.047	74.559		24.59
9 a sax	MOTA	2678	CD2	PHE A	340	33.902	40.592	72.616	1.00	28.22
	MOTA	2679	CE1	PHE A	340	35.063	41.330	75.072	1.00	21.58
₿«A»	ATOM	2680	CE2	PHE A	340	33.715	41.879	73.115	1.00	29.13
25	ATOM	2681	CZ	PHE A		34.280	42.225	74.345		25.28
25	ATOM	2682	N	ASN A		31.944	37.663	72.004		28.41
福養事 20		2683	CA.	ASN A		30.600		71.728		
41	ATOM						38.084			29.60
laft.	ATOM	2684	С	ASN A		29.665	37.110	72.379		38.52
選 (ATOM	2685	0	ASN A		28.699	37.511	73.029		42.88
71	MOTA	2686	CB	ASN A		30.322	38.274	70.224	1.00	30.01
30	MOTA	2687	CG	ASN A	341	31.159	39.374	69.587	1.00	52.80
ī.	ATOM	2688	OD1	ASN A	341	31.528	39.284	68.404	1.00	60.88
T.	MOTA	2689	ND2	ASN A	341	31.442	40.427	70.359	1.00	41.02
day.	ATOM	2690	N	ALA A		29.994	35.826	72.239		28.24
AN AND	ATOM	2691	CA	ALA A		29.195	34.800	72.877		26.95
35	ATOM	2692	C	ALA A		29.013	35.134	74.393		35.98
-k JJ		2693	0							
	ATOM			ALA A		27.877	35.261	74.897		35.09
	ATOM	2694	СВ	ALA A		29.837	33.422	72.671		25.45
	ATOM	2695	N	LEU A		30.153	35.304	75.122		29.16
	ATOM	2696	CA	LEU A		30.162	35.633	76.560	1.00	22.58
40	MOTA	2697	С	LEU A	343	29.310	36.854	76.831	1.00	27.48
	MOTA	2698	0	LEU A	343	28.452	36.821	77.696	1.00	32.73
	MOTA	2699	CB	LEU A	343	31.583	35.786	77.147	1.00	18.70
	ATOM	2700	CG	LEU A	343	31.647	35.693	78.671		20.08
	ATOM	2701		LEU A		30.842	34.510	79.204		17.76
45	ATOM	2702		LEU A		33.091	35.522	79.111		21.94
	ATOM	2703	N	GLY A		29.512	37.936	76.080		22.60
	ATOM	2704	CA			28.670	39.146	76.278		24.15
	MOTA	2705	С	GLY A		27.157	38.824	76.136		31.38
	MOTA	2706	0	GLY A		26.339	39.260	76.943	1.00	32.44
50	MOTA	2707	N	GLY A	345	26.806	38.017	75.094	1.00	22.79
	ATOM	2708	CA	GLY A	345	25.451	37.587	74.801	1.00	19.88
	ATOM	2709	С	GLY A		24.787	36.994	76.034		28.37
	ATOM	2710	0	GLY A		23.632	37.294	76.325		27.56
	ATOM	2711	N	TRP A		25.547	36.153	76.765		25.41
55	ATOM		CA							
, 55		2712		TRP A		25.082	35.520	77.994		23.90
	MOTA	2713	C	TRP A		24.825	36.541	79.071		31.54
	ATOM	2714	0	TRP A		23.957	36.379	79.924		29.57
	ATOM	2715	CB	TRP A		26.122	34.556	78.562		21.53
	ATOM	2716	CG	TRP A	346	25.680	33.880	79.837		21.92
60	ATOM	2717	CD1	TRP A	346	25.933	34.335	81.079		24.36
	ATOM	2718		TRP A		25.004	32.597	80.010		20.97
	ATOM	2719		TRP A		25.450	33.453			23.95
	ATOM	2720		TRP A		24.859	32.388	81.391		
									1.00	24.13
	MOTA	2721	CEO	TRP A	. 340	24.488	31.611	79.144	1.00	21.46

	MOTA	2722	CZ2	TRP A	346		24.225	31.244	81.921	1.00	22.89
	ATOM	2723	CZ3	TRP A	346		23.872	30.477	79.662		22.03
	ATOM	2724	CH2	TRP A	346		23.747	30.286	81.046		21.87
	ATOM	2725	N	GLY A			25.627	37.593	79.039		29.66
. 5	ATOM	2726	CA	GLY A			25.465	38.625	80.042		29.03
	MOTA	2727	С	GLY A			24.156	39.333	79.844		33.01
	MOTA	2728	0	GLY A		*	23.491	39.647	80.799		34.17
	ATOM	2729	N	GLU A			23.797	39.574	78.581		30.57
10	MOTA	2730	CA	GLU A			22.535	40.220	78.250		29.17
10	ATOM	2731	C	GLU A			21.423	39.282	78.664		31.25
	ATOM	2732	0	GLU A			20.373	39.663	79.142		33.71
	ATOM	2733	CB	GLU A			22.432	40.606	76.757		30.33
	ATOM	2734	CG	GLU A			23.432	41.715	76.336		49.41
1.5	ATOM	2735	CD	GLU A			23.209	43.088	76.964		73.39
15	ATOM	2736	OE1				22.295	43.846	76.656		71.22
	ATOM	2737		GLU A			24.119	43.395	77.857		44.23
	ATOM	2738	N	LEU A			21.682	38.011	78.541		27.36
92 m ,	ATOM	2739	CA	LEU A			20.677	37.081	78.976		26.89
20	ATOM	2740	С	LEU A			20.429	37.250	80.485		24.87
12 20	MOTA	2741	0	LEU A			19.299	37.403	80.914		28.31
u.	ATOM	2742	CB	LEU A			20.984	35.630	78.529		27.18
k.k.	ATOM	2743	CG	LEU A			19.943	34.565	78.942		32.45
17% 	ATOM	2744		LEU A			18.611	34.704	78.154	1.00	30.09
25	ATOM	2745		LEU A			20.541	33.169	78.749		27.10
23	ATOM	2746	N	GLN A			21.460	37.255	81.315	1.00	14.78
	ATOM	2747	CA	GLN A			21.188	37.428	82.727	1.00	18.51
 - 4.	ATOM	2748	C	GLN A			20.442	38.722	82.953		25.53
**	ATOM	2749	0	GLN A			19.495	38.833	83.737		28.35
30	ATOM	2750	CB	GLN A			22.469	37.369	83.536		22.22
	ATOM	2751	CG	GLN A			23.512	36.426	82.919		22.37
n.	ATOM	2752	CD	GLN A			24.871	36.673	83.547	1.00	34.49
12.0	ATOM	2753	OE1	GLN A			25.261	35.932	84.417		24.01
्रेस को इस को	ATOM	2754		GLN A			25.588	37.727	83.127		36.58
35	ATOM	2755	N	ASN A			20.838	39.696	82.201	1.00	22.64
<u>⊫</u> 35	ATOM	2756	CA	ASN A			20.163	40.960	82.273		26.10
	ATOM	2757	c	ASN A			18.661	40.780	82.083		37.49
	ATOM ATOM	2758 2759	O CB	ASN A			17.890	41.098	82.977		41.41
	ATOM	2760	CG	ASN A			20.769	42.021	81.341		20.74
40	ATOM	2761		ASN A			22.118	42.477	81.847		23.25
	ATOM	2762		ASN A			22.692	41.875	82.771		26.88
	ATOM	2763	N	SER A			22.644 18.228	43.530	81.247		32.93
	ATOM	2764	CA	SER A			16.784	40.252	80.938		32.84
	ATOM	2765	C	SER A			16.107	40.041 39.135	80.715		34.27
45	ATOM	2766	ŏ	SER A			14.927		81.784	1.00	31.72
	ATOM	2767	СВ	SER A			16.503	39.266 39.531	82.189 79.301		28.64
	ATOM	2768	OG	SER A			17.506	39.979	78.407		42.57
	ATOM	2769	N	VAL A			16.874	38.188	82.247		49.17
	ATOM	2770	CA	VAL A			16.322	37.351	83.234		21.90
50	ATOM	2771	С	VAL A			16.068	38.122	84.516		22.13 36.22
	ATOM	2772	0	VAL A			14.958	38.076	85.052		37.69
	ATOM	2773	CB	VAL A			17.137	36.070	83.419		20.84
	MOTA	2774		VAL A			16.632	35.256	84.634		15.06
	ATOM	2775		VAL A			16.968	35.284	82.105		20.93
55	ATOM	2776	N	LYS A			17.086	38.847	85.002		
	ATOM	2777	CA	LYS A			16.880	39.587	86.221		30.67 31.71
	ATOM	2778	C	LYS A			15.660	40.474	86.098		36.17
	ATOM	2779	0	LYS A			14.808	40.582	86.980		35.80
	ATOM	2780	CB	LYS A			18.099	40.396	86.624		35.28
60	MOTA	2781	CG	LYS A			17.841	41.303	87.818		51.51
	ATOM	2782	CD	LYS A			19.038	41.405	88.749		60.46
	MOTA	2783	CE	LYS A			19.198	42.780	89.383	1.00	50.46
	ATOM	2784	NZ	LYS A			20.596	43.133	89.657		63.77
	MOTA	2785	N	THR A			15.608	41.108	84.962		32.63

		2001	2206	C 3	mun a		255	14 560	40 005	04 630	1 00 24 02
		MOTA	2786		THR A			14.562	42.025	84.610	1.00 34.03
		MOTA	2787		THR A			13.129	41.422	84.578	1.00 42.11
		ATOM	2788		THR A			12.216	42.006	85.154	1.00 40.96
		ATOM	2789		THR A			14.974	42.736	83.308	1.00 41.11
	5	ATOM	2790		THR A			16.071	43.615	83.542	1.00 29.85
	1	ATOM	2791		THR A			13.798	43.438	82.656	1.00 45.50
		MOTA	2792		PHE A			12.895	40.273	83.908	1.00 33.89
		MOTA	2793		PHE A			11.556	39.729	83.860	1.00 29.29
	10	ATOM	2794		PHE A			11.209	39.070	85.147	1.00 31.93
	10	ATOM	2795		PHE A			10.089	39.152	85.642	1.00 33.85
		ATOM	2796	CB	PHE A			11.460	38.645	82.785	1.00 33.30
		ATOM	2797	CG	PHE A			11.187	39.196	81.416	1.00 36.54
		MOTA	2798		PHE A			10.106	40.054	81.224	1.00 42.38
	1.5	MOTA	2799		PHE A			11.985	38.858	80.320	1.00 38.62
	15	MOTA	2800		PHE A			9.831	40.596	79.968	1.00 44.75
		ATOM	2801		PHE A			11.723	39.384	79.055	1.00 43.46
		ATOM	2802	CZ	PHE A			10.649	40.261	78.890	1.00 43.86
		ATOM	2803	N	GLY A			12.212	38.386	85.661	1.00 30.41
10 10		ATOM	2804	CA	GLY A			12.152	37.564	86.864	1.00 29.17
nie.	20	MOTA	2805	С	GLY A			12.446	36.100	86.438	1.00 28.92
H.		MOTA	2806	0	GLY A			12.008	35.642	85.372	1.00 27.33
in the		ATOM	2807	N	GLU A			13.211	35.382	87.243	1.00 21.27
		ATOM	2808	CA	GLU A	ł	358	13.590	34.040	86.898	1.00 23.10
THE MILE		MOTA	2809	С	GLU A			12.424	33.104	86.747	1.00 31.53
अर्थे कर्	25	MOTA	2810	0	GLU A	1	358	12.581	31.972	86.294	1.00 30.92
		MOTA	2811	CB	GLU A	¥	358	14.596	33.473	87.880	1.00 25.36
}= ₽0		MOTA	2812	CG	GLU A	Ą	358	14.011	33.436	89.301	1.00 38.73
*		MOTA	2813	CD	GLU A	ł	358	15.011	33.037	90.345	1.00 56.34
na in		ATOM	2814	OE1	GLU A	ł	358	16.026	32.446	90.071	1.00 50.55
वास्त्र अस्त्र साम्राज्य	30	ATOM	2815	OE2	GLU A	4	358	14.678	33.403	91.564	1.00 75.65
T.		MOTA	2816	N	THR A	A.	359	11.246	33.542	87.139	1.00 27.87
		MOTA	2817	CA	THR A	Ą.	359	10.154	32.625	86.970	1.00 25.66
12.00		ATOM	2818	С	THR A	Į.	359	9.236	33.152	85.906	1.00 25.96
122		ATOM	2819	0	THR A	4	359	8.247	32.528	85.533	1.00 25.58
i se	35	ATOM	2820	CB	THR A	Ą	359	9.423	32.341	88.253	1.00 25.00
11-3-2		ATOM	2821	OG1	THR A	4	359	8.908	33.565	88.692	1.00 33.10
		ATOM	2822	CG2	THR A	4	359	10.406	31.785	89.273	1.00 14.43
		ATOM	2823	N	HIS A	A.	360	9.602	34.310	85.407	1.00 20.75
		ATOM	2824	CA	HIS A	4	360	8.837	34.902	84.363	1.00 22.77
	40	ATOM	2825	C	HIS A	4	360	8.823	34.034	83.130	1.00 35.30
		MOTA	2826	0	HIS A	Ą	360	9.858	33.611	82.620	1.00 37.42
		MOTA	2827	CB	HIS A	4	360	9.294	36.291	83.982	1.00 23.18
		ATOM	2828	CG	HIS A	Ą.	360	8.207	36.908	83.219	1.00 27.05
	1	ATOM	2829	ND1	HIS A	4	360	7.532	38.009	83.691	1.00 29.34
	45	ATOM	2830	CD2	HIS A	Ą	360	7.651	36.545	82.059	1.00 29.91
		MOTA	2831	CE1	HIS A	4	360	6.596	38.315	82.806	1.00 27.94
		MOTA	2832	NE2	HIS A	4	360	6.651	37.440	81.812	1.00 29.60
		MOTA	2833	N	PRO A	Ą	361	7.606	33.817	82.666	1.00 32.40
		MOTA	2834	CA	PRO A			7.301	32.999	81.519	1.00 29.46
	50	ATOM	2835	C	PRO A	Ą	361	7.862	33.478	80.224	1.00 30.59
		MOTA	2836	0	PRO A	4	361	7.907	32.737	79.248	1.00 33.00
		ATOM	2837	CB	PRO A			5.770	32.963	81.478	1.00 30.74
		ATOM	2838	CG	PRO A	Ą	361	5.311	33.172	82.927	1.00 34.96
	-	MOTA	2839	CD	PRO A	A	361	6.463	33.869	83.627	1.00 31.82
	55	MOTA	2840	N	PHE 2	A	362	8.289	34.712	80.179	1.00 26.32
		MOTA	2841	CA	PHE I			8.823	35.173	78.933	1.00 25.68
		ATOM	2842	C	PHE I	A	362	10.261	34.781	78.829	1.00 29.73
		MOTA	2843	0	PHE 2	A	362	10.906	35.131	77.870	1.00 32.02
		ATOM	2844	CB	PHE I			8.643	36.677	78.723	1.00 28.12
	60	ATOM	2845	CG	PHE I			7.194	37.105	78.629	1.00 30.03
		MOTA	2846	CD1	PHE I			6.204	36.276	78.098	1.00 30.92
		MOTA	2847		PHE 2				38.372	79.051	1.00 32.04
		ATOM	2848		PHE			4.864	36.655	77.998	1.00 26.59
		ATOM	2849		PHE			5.470	38.773	78.952	1.00 32.40

	ATOM	2914	С	ASP A 371	-2.557	37.636	75.255	1.00 40.92
	MOTA	2915		ASP A 371	-2.784	38.625	75.933	1.00 41.63
	MOTA	2916		ASP A 371	-4.519	36.375	76.245	1.00 39.88
	MOTA	2917		ASP A 371	-5.805	35.733	75 .7 98	1.00 51.30
. 5	ATOM	2918	OD1	ASP A 371	-6.373	36.072	74.761	1.00 50.39
	ATOM	2919	OD2	ASP A 371	-6.206	34.754	76.583	1.00 48.61
	ATOM	2920	N	ILE A 372.	-1.387	37.398	74.664	1.00 36.37
	ATOM	2921	CA	ILE A 372	-0.259	38.283	74.817	1.00 34.61
	MOTA	2922	C	ILE A 372	0.203	39.018	73.555	1.00 35.46
10	MOTA	2923	0	ILE A 372	0.545	38.400	72.548	1.00 36.69
	MOTA	2924	CB	ILE A 372	0.920	37.511	75.381	1.00 36.51
	ATOM	2925			0.658	37.195	76.842	1.00 37.01
	MOTA	2926		ILE A 372	2.121	38.441	75.281	1.00 35.52
	MOTA	2927	CD1	ILE A 372	1.268	38.261	77.747	1.00 54.33
15	MOTA	2928	N	ASP A 373	0.254	40.345	73.601	1.00 25.92
	MOTA	2929	CA	ASP A 373	0.747	41.053	72.450	1.00 23.77
	ATOM	2930	С	ASP A 373	2.263	40.781	72.360	1.00 31.40
	ATOM	2931	0	ASP A 373	3.040	41.002	73.305	1.00 32.80
20	ATOM	2932	CB	ASP A 373	0.408	42.543	72.519	1.00 25.08
20	ATOM	2933	CG	ASP A 373	1.064	43.356	71.418	1.00 43.24
	MOTA	2934		ASP A 373	1.861	42.894	70.616	1.00 45.30
	MOTA	2935		ASP A 373	0.668	44.610	71.395	1.00 38.59
	MOTA	2936	N	PRO A 374	2.709	40.267	71.225	1.00 29.51
0.5	MOTA	2937	CA	PRO A 374	4.123	39.943	71.132	1.00 28.52
25	ATOM	2938	С	PRO A 374	5.029	41.090	71.506	1.00 32.54
	ATOM	2939	0	PRO A 374	6.019	40.905	72.217	1.00 29.62
	ATOM	2940	CB	PRO A 374	4.390	39.421	69.714	1.00 28.88
	MOTA	2941	CG	PRO A 374	3.028	39.278	69.032	1.00 32.27
20	ATOM	2942	CD	PRO A 374	1.966	39.786	70.008	1.00 28.84
30	ATOM	2943	N	ASP A 375	4.660	42.257	70.981	1.00 26.85
	ATOM	2944	CA	ASP A 375	5.357	43.511	71.154	1.00 24.25
	ATOM	2945	C	ASP A 375 ASP A 375	5.695 6.648	43.783 44.494	72.628 72.988	1.00 33.10
	ATOM ATOM	2946 2947	O CB	ASP A 375	4.507	44.494	70.509	1.00 30.67 1.00 24.46
35	ATOM	2948	CG	ASP A 375	4.753	44.836	69.033	1.00 24.40
33	ATOM	2949		ASP A 375	5.703	44.393	68.411	1.00 30.08
	ATOM	2950		ASP A 375	3.852	45.609	68.491	1.00 38.41
	ATOM	2951	N	VAL A 376	4.885	43.161	73.477	1.00 30.21
	ATOM	2952	CA	VAL A 376	5.001	43.232	74.904	1.00 25.40
40	ATOM	2953	c	VAL A 376	5.879	42.106	75.431	1.00 37.27
	MOTA	2954	ō	VAL A 376	6.599	42.299	76.394	1.00 42.46
	ATOM	2955	CB	VAL A 376	3.638	43.099	75.550	1.00 22.48
	ATOM	2956		VAL A 376	3.799	42.533	76.975	1.00 21.25
	ATOM	2957		VAL A 376	2.926	44.440	75.547	1.00 18.29
45	ATOM	2958	N	ALA A 377	5.811	40.905	74.831	1.00 30.48
	ATOM	2959	CA	ALA A 377	6.671	39.793	75,288	1.00 27.04
	ATOM	2960	С	ALA A 377	8.149	39.911	74.797	1.00 28.15
	ATOM	2961	0	ALA A 377	9.077	39.325	75.312	1.00 27.36
1	MOTA	2962	CB	ALA A 377	6.091	38.433	74.891	1.00 26.74
50	ATOM	2963	N	TYR A 378	8.376	40.692	73.768	1.00 25.81
	ATOM	2964	CA	TYR A 378	9.683	40.876	73.161	1.00 25.43
	MOTA	2965	С	TYR A 378	10.862	41.194	74.057	1.00 30.49
	ATOM	2966	0	TYR A 378	10.873	42.204	74.747	1.00 32.35
	ATOM	2967	CB	TYR A 378	9.549	41.924	72.068	1.00 26.20
55	ATOM	2968	CG	TYR A 378	10.804	42.168	71.327	1.00 19.90
	ATOM	2969		TYR A 378	11.256	41.231	70.406	1.00 18.53
	ATOM	2970		TYR A 378	11.536	43.331	71.543	1.00 18.47
	ATOM	2971		TYR A 378	12.444	41.436	69.716	1.00 15.98
60	MOTA	2972		TYR A 378	12.719	43.555	70.840	1.00 18.77
60	ATOM	2973	CZ	TYR A 378	13.161	42.609	69.920	1.00 16.37
	ATOM	2974	OH	TYR A 378	14.309	42.811	69.212	1.00 32.30
	ATOM	2975	N	SER A 379	11.879	40.317	73.977	1.00 23.03
	ATOM	2976	CA	SER A 379	13.115	40.430	74.725	1.00 18.13
	ATOM	2977	C	SER A 379	14.267	39.777	73.970	1.00 20.60

The first of the f

		ATOM	2850	CZ	PHE A	362	4.495	37.920	78.435	1.00 26.37
		ATOM	2851	N	THR A	363	10.730	34.049	79.843	1.00 27.22
		ATOM	2852	CA	THR A		12.102	33.575	79.943	1.00 27.52
			2853	C						
		MOTA			THR A		12.251	32.132	79.504	1.00 29.28
	5	ATOM	2854	0	THR A		13.331	31.560	79.524	1.00 29.42
		ATOM	2855	CB	THR A	363	12.697	33.777	81.360	1.00 31.67
		ATOM	2856	OG1	THR A	363	12.279	32.745	82.218	1.00 26.17
		MOTA	2857	CG2	THR A	363	12.278	35.118	81.930	1.00 31.62
		ATOM	2858	N	LYS A		11.148	31.530	79.113	1.00 23.08
	10		2859	CA						
	10	ATOM			LYS A		11.174	30.160	78.664	1.00 20.50
		MOTA	2860	С	LYS A		11.556	30.270	77.217	1.00 28.83
		ATOM	2861	0	LYS A	364	11.139	31.239	76.570	1.00 29.80
		MOTA	2862	CB	LYS A	364	9.766	29.584	78.667	1.00 23.55
		ATOM	2863	CG	LYS A	364	9.252	29.134	80.022	1.00 40.85
	15	ATOM	2864	CD	LYS A		7.761	29.369	80.162	
	10			CE						1.00 44.83
		MOTA	2865		LYS A		7.131	28.492	81.224	1.00 66.38
		ATOM	2866	NZ	LYS A		6.063	27.638	80.691	1.00 91.70
	1	ATOM	2867	N	LEU A	365	12.332	29.328	76.698	1.00 23.57
		MOTA	2868	CA	LEU A	365	12.699	29.420	75.312	1.00 23.95
	20	MOTA	2869	С	LEU A	365	11.414	29.419	74.445	1.00 35.57
रीई और		ATOM	2870	0	LEU A		11.166	30.369	73.708	
Hand.										1.00 34.58
Bay Sho		MOTA	2871	CB	LEU A		13.702	28.303	75.021	1.00 25.08
magnet.		 MOTA	2872	CG	LEU A		14.456	28.372	73.702	1.00 31.15
e aur		ATOM	2873		LEU A		14.987	29.778	73.466	1.00 33.16
1784 1785	25	ATOM	2874	CD2	LEU A	365	15.609	27.353	73.781	1.00 30.62
L.		ATOM	2875	N	VAL A		10.572	28.360	74.564	1.00 35.62
G= 4.		ATOM	2876	CA	VAL A		9.294	28.232	73.840	
FTTT										1.00 32.10
學		ATOM	2877	C	VAL A		8.211	28.911	74.694	1.00 33.14
in the	-	ATOM	2878	0	VAL A		7.982	28.470	75.808	1.00 34.20
The second	30	MOTA	2879	CB	VAL A		8.936	26.739	73.568	1.00 34.73
1 (m)		ATOM	2880	CG1	VAL A	366	7.558	26.605	72.933	1.00 34.88
		MOTA	2881		VAL A		9.922	26.012	72.649	1.00 32.65
12 tr		ATOM	2882	N	VAL A		7.562	29.990	74.211	1.00 28.76
the stiff			2883	CA						
22	25	ATOM			VAL A		6.532	30.700	74.987	1.00 28.27
1	35	MOTA	2884	С	VAL A		5.161	30.613	74.420	1.00 30.62
-		ATOM	2885	0	VAL A	367	4.994	30.509	73.235	`1.00 34.30
		ATOM	2886	CB	VAL A	367	6.773	32.185	75.061	1.00 33.45
		MOTA	2887	CG1	VAL A	367	8.178	32.478	75.565	1.00 33.03
		ATOM	2888		VAL A		6.498	32.804	73.693	1.00 33.18
	40	ATOM	2889	N	ASP A		4.168	30.722	75.290	
		ATOM	2890	CA	ASP A					1.00 29.27
							2.764	30.771	74.984	1.00 27.67
		ATOM	2891	С	ASP A		2.315	32.207	74.862	1.00 26.94
		ATOM	2892	0	ASP A	368	2.283	32.975	75.830	1.00 23.11
	× 1.0	MOTA	2893	CB	ASP A	368	1.990	30.073	76.100	1.00 26.80
	45	ATOM	2894	CG	ASP A	368	0.572	29.781	75.613	1.00 37.90
		ATOM	2895		ASP A		0.276	30.123	74.481	1.00 38.93
		ATOM	2896		ASP A		-0.215	29.217	76.380	1.00 38.59
		ATOM	2897	N	LEU A					
							2.027	32.588	73.622	1.00 26.55
	50	MOTA	2898	CA	LEU A		1.643	33.953	73.373	1.00 27.39
	50	ATOM	2899	С	LEU A		0.138	34.105	73.301	1.00 30.74
		ATOM	2900	0	LEU A	369	-0.372	34.979	72.648	1.00 30.68
		ATOM	2901	CB	LEU A	369	2.281	34.395	72.064	1.00 26.06
:27		ATOM	2902	CG	LEU A		3.759	34.760	72.229	1.00 26.80
		ATOM	2903		LEU A		4.343	35.415	70.994	1.00 24.30
	55		2904		LEU A					
	25	ATOM					4.014	35.728	73.384	1.00 21.81
		ATOM	2905	N	THR A		-0.577	33.154	73.953	1.00 30.26
		MOTA	2906	CA	THR A		-2.022	33.306	74.093	1.00 31.38
		ATOM	2907	С	THR A	370	-2.355	34.519	74.941	1.00 38.62
		ATOM	2908	0	THR A		-1.821	34.714	76.027	1.00 38.84
	60	ATOM	2909	CB	THR A		-2.601	32.056	74.750	1.00 34.04
		ATOM	2910		THR A		-2.472			
								30.949	73.873	1.00 29.99
		ATOM	2911		THR A		-4.091	32.266	75.052	1.00 26.40
		MOTA	2912	N	ASP A		-3.173	35.387	74.363	1.00 37.89
		ATOM	2913	CA	ASP A	371	-3.641	36.612	75.012	1.00 37.85

m #12
144
ga 🌬
12 m:
研究
14
12
1-4
1
122

	ATOM	2978	0	SER A	379	14.100	39.334	72.843	1.00 18.46
	ATOM	2979	CB	SER A	379	12.976	39.740	76.067	1.00 23.56
	MOTA	2980	OG	SER A	379	12.805	38.329	75.883	1.00 37.26
_	MOTA	2981	N	SER A	380	15.424	39.697	74.651	1.00 23.65
5	MOTA	2982	CA	SER A		16.701	39.084	74.222	1.00 26.09
	MOTA	2983	C	SER A		16.669	37.571	74.457	1.00 28.37
	ATOM	2984	0	SER A		17.480	36.785	73.975	1.00 30.81
	ATOM	2985	CB	SER A		17.889	39.588	75.062	1.00 31.60
	ATOM	2986	OG	SER A		18.036	41.000	75.033	1.00 42.48
10	MOTA	2987	И	VAL A		15.718	37.188	75.260	1.00 18.04
	ATOM	2988	CA	VAL A		15.595	35.812	75.598	1.00 14.91
	ATOM	2989	C	VAL A		15.708	34.897	74.419	1.00 20.31
	ATOM	2990	0	VAL A		16.620	34.091	74.330	1.00 27.64
1.5	MOTA	2991	CB	VAL A		14.408	35.546	76.501	1.00 16.34
15	ATOM	2992		VAL A		14.284	34.062	76.734	1.00 17.26
	MOTA	2993		VAL A		14.687	36.204	77.829	1.00 13.94
	MOTA	2994	N	PRO A		14.797	35.005	73.489	1.00 16.53
	ATOM	2995	CA	PRO A		14.886	34.139	72.324	1.00 17.21
20	ATOM	2996	С	PRO A		16.222	34.230	71.634	1.00 24.01
20	ATOM	2997	0	PRO A		16.709	33.192	71.207	1.00 27.79
	ATOM	2998	CB	PRO A		13.777	34.514	71.351	1.00 17.20
	MOTA	2999	CG	PRO A		13.003	35.618	72.033	1.00 18.32
	ATOM	3000	CD	PRO A		13.627	35.873	73.399	1.00 12.12
25	ATOM	3001	N	TYR A		16.809	35.447	71.542	1.00 19.33
25	MOTA	3002	CA	TYR A		18.112	35.648	70.902	1.00 19.70
	ATOM	3003	C	TYR A		19.246	34.953	71.651	1.00 28.79
	ATOM	3004	O	TYR A		19.980	34.117	71.104	1.00 31.38
	ATOM	3005 3006	CB	TYR A		18.468	37.135	70.894	1.00 21.02
30	MOTA	3007	CG CD1	TYR A		17.593	37.968	70.011	1.00 23.86
30	ATOM ATOM	3007		TYR A		16.290 18.067	38.277 38.450	70.404	1.00 28.36 1.00 20.93
	ATOM	3009		TYR A		15.473	39.054	68.784 69.576	1.00 20.93
	ATOM	3010		TYR A		17.272	39.244	67.957	1.00 30.88
	ATOM	3010	CZ	TYR A		15.967	39.533	68.358	1.00 18.71
 35	ATOM	3012	OH	TYR A		15.171	40.294	67.556	1.00 20.33
	ATOM	3013	N	GLU A		19.389	35.333	72.921	1.00 20.17
	ATOM	3014	CA	GLU A		20.419	34.857	73.803	1.00 17.57
	ATOM	3015	С	GLU A		20.188	33.506	74.405	1.00 22.88
	ATOM	3016	0	GLU A		21.151	32.775	74.669	1.00 25.65
40	ATOM	3017	CB	GLU A	384	20.833	35.973	74.773	1.00 20.44
	ATOM	3018	CG	GLU A	384	21.263	37.202	73.944	1.00 15.21
	ATOM	3019	CD	GLU A	384	22.539	36.937	73.184	1.00 26.58
	ATOM	3020	OE1	GLU A	384	23.185	35.915	73.293	1.00 17.84
	MOTA	3021		GLU A		22.887	37.915	72.400	1.00 21.88
45	ATOM	3022	N	LYS A		18.935	33.116	74.610	1.00 20.33
	ATOM	3023	CA	LYS A		18.736	31.767	75.146	1.00 20.05
	ATOM	3024	С	LYS A		18.865	30.716	74.028	1.00 27.19
	ATOM	3025	0	LYS A		19.420	29.621	74.219	1.00 31.66
50	ATOM	3026	CB	LYS A		17.507	31.577	76.014	1.00 21.51
50	ATOM	3027	CG	LYS A		17.676	30.384	76.953	1.00 22.29
	ATOM	3028	CD	LYS A		16.386	29.820	77.518	1.00 19.87
	MOTA	3029	CE	LYS A		16.049	30.277	78.937	1.00 31.60
	ATOM	3030	NZ	LYS A		14.783	29.694	79.441	1.00 30.38
55	ATOM	3031	N	GLY A		18.364	31.084	72.832	1.00 20.72
55	MOTA	3032	CA	GLY A		18.453	30.248	71.637	1.00 17.41
	ATOM	3033	C	GLY A		19.924	30.106	71.298	1.00 20.81
	ATOM	3034	N O			20.396	29.001	71.225	1.00 22.50
	ATOM ATOM	3035 3036	CA.	PHE A		20.683 22.137	31.228	71.163	1.00 20.30
60	MOTA	3036	CA	PHE A		22.137	31.158 30.263	70.900	1.00 19.92
00	ATOM	3037	0	PHE A		23.685	29.478	71.905 71.530	1.00 29.09 1.00 32.80
	ATOM	3039	СВ	PHE A		22.852	32.519	70.955	1.00 32.80
	MOTA	3040	CG	PHE A		24.344	32.319	70.933	1.00 20.07
	ATOM	3041		PHE A		24.949	32.163	69.631	1.00 19.67
			1						

		ATOM	3042	CD2	PHE A	387	25.157	32.373	72.007	1.00 25.27
		ATOM	3043		PHE A		26.329	31.977	69.525	1.00 20.88
		ATOM	3044	CE2	PHE A	387	26.542	32.202	71.916	1.00 28.83
		ATOM	3045	CZ	PHE A	387	27.131	31.981	70.668	1.00 23.24
	5	MOTA	3046	N	ALA A	388	22.495	30.381	73.203	1.00 25.48
		MOTA	3047	CA	ALA A	388	23.133	29.556	74.242	1.00 23.14
		ATOM	3048	С	ALA A	388	22.872	28.108	74.055	1.00 32.10
		ATOM	3049	0	ALA A		23.757	27.282	74.258	1.00 37.82
		ATOM	3050	CB	ALA A		22.717	29.932	75.633	1.00 23.02
	10	MOTA	3051	N .	LEU A		21.636	27.793	73.691	1.00 26.31
		ATOM	3052	CA	LEU A		21.275	26.405	73.460	1.00 21.42
		MOTA	3053	C	LEU A		22.189	25.906	72.372	1.00 27.91
		MOTA	3054	0	LEU A		22.865	24.900	72.532	1.00 29.25
	15	MOTA	3055	CB	LEU A		19.841	26.300	72.937	1.00 19.24
	13	MOTA	3056	CG	LEU A		19.427	24.868	72.632	1.00 17.17
		MOTA	3057 3058		LEU A		19.717 17.943	24.017 24.808	73.844	1.00 14.63
		ATOM ATOM	3059	N N	LEU A		22.217	26.659	72.328	1.00 10.16
		ATOM	3060	CA	LEU A		23.050	26.340	71.262 70.107	1.00 24.49 1.00 25.05
	20	ATOM	3061	C	LEU A		24.531	26.256	70.383	1.00 23.03
	20	ATOM	3062	0	LEU A		25.183	25.301	69.932	1.00 32.31
4		ATOM	3063	CB	LEU A		22.765	27.152	68.844	1.00 33.00
je ik		ATOM	3064	CG	LEU A		21.307	27.026	68.442	1.00 23.38
18 B. S.		ATOM	3065		LEU A		20.986	28.025	67.334	1.00 20.84
1990 1990	25	ATOM	3066		LEU A		20.988	25.591	68.017	1.00 18.86
LTS.		ATOM	3067	N	PHE A		25.058	27.231	71.127	1.00 28.52
H= 50		ATOM	3068	CA	PHE A		26.480	27.236	71.494	1.00 27.82
		ATOM	3069	С	PHE A		26.813	25.992	72.312	1.00 28.67
1-5		MOTA	3070	0	PHE A	391	27.839	25.331	72.148	1.00 26.96
n,	30	MOTA	3071	CB	PHE A	391	26.834	28.455	72.341	1.00 28.60
		MOTA	3072	CG	PHE A	391	28.296	28.786	72.283	1.00 30.53
n.		MOTA	3073	CD1	PHE A	391	28.967	28.816	71.064	1.00 35.08
		MOTA	3074		PHE A		29.020	29.063	73.440	1.00 36.52
	2.5	MOTA	3075		PHE A		30.320	29.142	70.983	1.00 37.61
	35	MOTA	3076		PHE A		30.378	29.383	73.382	1.00 40.61
		ATOM	3077	CZ	PHE A		31.026	29.432	72.148	1.00 37.64
		ATOM	3078	N	TYR A		25.913	25.699	73.225	1.00 24.90
		ATOM	3079 3080	CA	TYR A		26.044	24.550 23.298	74.065	1.00 24.66
	40	ATOM ATOM	3081	C O	TYR A		26.106 27.058	22.558	73.186	1.00 34.30 1.00 37.51
	70	ATOM	3082	CB	TYR A		24.821	24.501	73.268 74.967	1.00 37.31
		ATOM	3083	CG	TYR A		24.631	23.181	75.678	1.00 20.39
		ATOM	3084		TYR A		25.546	22.715	76.625	1.00 35.17
		ATOM	3085		TYR A		23.501	22.397	75.432	1.00 32.49
	45	ATOM	3086		TYR A		25.341			1.00 39.01
		ATOM	3087	CE2	TYR A	392	23.281	21.184	76.094	1.00 31.50
		ATOM	3088	CZ	TYR A	392	24.206	20.743	77.035	1.00 34.08
		ATOM	3089	OH	TYR A		23.986	19.564	77.683	1.00 36.46
	-	MOTA	3090	N	LEU A		25.101	23.067	72.310	1.00 31.02
	50	MOTA	3091	CA	LEU A		25.043	21.889	71.410	1.00 29.65
		MOTA	3092	С	LEU A		26.274	21.616	70.507	1.00 32.03
		ATOM	3093	0	LEU A		26.664	20.468	70.267	1.00 27.90
		ATOM	3094	CB	LEU A		23.758	21.905	70.552	1.00 28.85
	55	ATOM	3095	CG	LEU A		22.489	21.688	71.375	1.00 30.33
	22	ATOM	3096		LEU A		21.256	22.047	70.559	1.00 27.38
		ATOM	3097		LEU A		22.400	20.246	71.865	1.00 29.76
		ATOM	3098	N CA	GLU A		26.841	22.701	69.980	1.00 30.84
	1	ATOM ATOM	3099 3100	CA C	GLU A		28.000 29.210	22.727 22.214	69.118	1.00 30.05
	60	ATOM	3100	0	GLU A		30.089	21.595	69.868 69.299	1.00 39.16 1.00 42.14
	- 50	ATOM	3102	СВ	GLU A		28.300	24.204	68.756	1.00 42.14
		ATOM	3103	CG	GLU A		29.776	24.406	68.376	1.00 31.03
		ATOM	3104	CD	GLU A		30.182	25.830	68.208	1.00 45.20
		ATOM	3105		GLU A		29.614	26.609	67.471	1.00 56.77
		*			-	-			- · · · - ·	

		ATOM	3106	OE2	GLU A	394	31.229	26.133	68.927	1.00 39.77
		ATOM	3107		GLN A		29.256	22.534	71.160	1.00 34.20
		ATOM	3108		GLN A		30.342	22.139	72.029	1.00 32.86
			_					20.690	72.435	1.00 32.00
	~	ATOM	3109		GLN A		30.143			
	5	ATOM	3110		GLN A		31.066	19.899	72.507	1.00 38.67
		MOTA	3111	CB	GLN A	395	30.474	23.051	73.287	1.00 33.17
		ATOM	3112	CG	GLN A	395	30.831	24.540	72.996	1.00 13.79
		ATOM	3113	CD	GLN A	395	31.176	25.354	74.247	1.00 37.45
		ATOM	3114		GLN A		30.909	24.959	75.407	1.00 26.89
	10				GLN A					1.00 20.09
	10	ATOM	3115				31.758	26.523	74.010	
		MOTA	3116		LEU A		28.903	20.352	72.682	1.00 38.68
		MOTA	3117	CA	LEU A	396	28.514	19.015	73.083	1.00 38.49
	114	MOTA	3118	C	LEU A	396	28.633	18.017	71.924	1.00 39.28
		MOTA	3119	0	LEU A	396	29.012	16.871	72.100	1.00 42.17
	15	MOTA	3120		LEU A		27.055	19.072	73.628	1.00 37.93
	15									
		ATOM	3121		LEU A		26.389	17.732	73.946	1.00 42.72
		MOTA	3122		LEU A		26.436	17.489	75.445	1.00 45.42
		MOTA	3123	CD2	LEU A		24.917	17.709	73.527	1.00 43.81
in all		MOTA	3124	N	LEU A	397	28.303	18.456	70.730	1.00 28.48
	20	MOTA	3125	CA	LEU A	397	28.337	17.595	69.589	1.00 25.49
1257		MOTA	3126	С	LEU A		29.620	17.609	68.771	1.00 36.86
ii.										
44		MOTA	3127	0	LEU A		29.596	17.220	67.599	1.00 39.85
		MOTA	3128	CB	LEU A		27.156	17.924	68.686	1.00 23.73
2 days		MOTA	3129	CG	LEU A	397	25.843	17.773	69.401	1.00 25.82
	25	MOTA	3130	CD1	LEU A	397	24.740	18,559	68.669	1.00 22.99
		ATOM	3131	CD2	LEU A	397	25.525	16.272	69.452	1.00 27.30
ind.		MOTA	3132	N	GLY A		30.731	18.069	69.342	1.00 33.98
				CA	GLY A		31.993	18.038	68.617	1.00 33.30
¥.		MOTA	3133							
hot.	•	MOTA	3134	С	GLY A		32.547	19.260	67.889	1.00 38.92
	30	ATOM	3135	0	GLY A		33.502	19.097	67.115	1.00 39.98
11 THE		MOTA	3136	N	GLY A	399	32.001	20.457	68.105	1.00 33.01
		ATOM	3137	CA	GLY A	399	32.543	21.650	67.440	1.00 30.35
14 mg		ATOM	3138	С	GLY A	399	31.713	22.336	66.365	1.00 31.72
12.20		MOTA	3139	ŏ	GLY A		30.800	21.823	65.762	1.00 34.57
केंद्र अर्थ	25									
la de	35	ATOM	3140	N	PRO A		32.076	23.550	66.124	1.00 33.01
		ATOM	3141	CA	PRO A		31.429	24.406	65.151	1.00 35.02
		ATOM	3142	С	PRO A	400	31.379	23.794	63.750	1.00 43.93
		ATOM	3143	0	PRO A	400	30.360	23.838	63.045	1.00 40.14
		ATOM	3144	CB	PRO A	400	32.293	25.672	65.111	1.00 35.73
	40	ATOM	3145	CG	PRO A		33.539	25.411	65.948	1.00 38.03
	10		3146	CD	PRO A			24.010	66.517	1.00 33.92
		MOTA					33.423			
		MOTA	3147	N	GLU A		32.512	23.237	63.345	1.00 43.85
		ATOM	3148	CA	GLU A		32.597	22.620	62.042	1.00 42.92
	0_0	ATOM	3149	С	GLU A	401	31.491	21.587	61.878	1.00 37.92
	45	ATOM	3150	0	GLU A	401	30.810	21.588	60.866	1.00 33.79
		ATOM	3151	CB	GLU A	401	33.996	22.034	61.789	1.00 45.93
		ATOM	3152	CG	GLU A		34.578	22.372	60.398	1.00 69.62
		ATOM	3153	CD	GLU A		35.603	21.373	59.911	1.00100.00
		,								
	50	ATOM	3154		GLU A		36.702	21.236	60.427	1.00100.00
	50	ATOM	3155	OE2	GLU A		35.195	20.689	58.865	1.00 93.16
		ATOM	3156	N	ILE A	402	31.317	20.720	62.902	1.00 34.58
		ATOM	3157	CA	ILE A	402	30.281	19.681	62.922	1.00 33.20
		ATOM	3158	С	ILE A	402	28.898	20.291	62.938	1.00 39.09
		ATOM	3159	ō	ILE A		28.065	19.896	62.133	1.00 41.43
	55									
	23	MOTA	3160	CB	ILE A		30.391	18.673	64.078	1.00 33.82
		MOTA	3161		ILE A		31.490	17.661	63.811	1.00 34.70
		MOTA	3162	CG2	ILE A	402	29.080	17.900	64.287	1.00 23.32
		ATOM	3163	CD1	ILE A	402	31.878	16.896	65.080	1.00 49.20
		ATOM	3164	N	PHE A		28.668	21.246	63.868	1.00 32.73
	60	ATOM	3165	CA	PHE A		27.390	21.952	64.044	1.00 29.52
	5.0									
		ATOM	3166	С	PHE A		27.032	22.816	62.836	1.00 33.94
		MOTA	3167	0	PHE A		25.866	23.022	62.469	1.00 34.15
		MOTA	3168	CB	PHE A		27.319	22.719	65.381	1.00 29.03
		ATOM	3169	CG	PHE A	403	25.917	22.783	65.929	1.00 28.54

		ATOM	3170	CD1	PHE A	403	25.323	21.643	66.484	1.00 29.91
		ATOM	3171		PHE A		25.176	23.964	65.873	1.00 27.62
			3172							
		MOTA			PHE A		24.021	21.667	66.990	1.00 27.38
	_	MOTA	3173		PHE A		23.881	24.017	66.393	1.00 28.82
	5	ATOM	3174	CZ	PHE A		23.304	22.863	66.932	1.00 25.72
		ATOM	3175	N	LEU A	404	28.040	23.327	62.165	1.00 31.31
		ATOM	3176	CA	LEU A	404	27.687	24.080	60.983	1.00 32.95
		ATOM	3177	C	LEU A		27.068	23.099	59.952	1.00 32.89
	10	ATOM	3178	0	LEU A		26.050	23.361	59.315	1.00 37.36
	10	ATOM	3179	СВ	LEU A		28.798	25.045	60.464	1.00 33.15
		ATOM	3180	CG	LEU A	404	29.029	26.208	61.444	1.00 36.96
		ATOM	3181	CD1	LEU A	404	30.454	26.717	61.353	1.00 37.13
		ATOM	3182	CD2	LEU A	404	28.083	27.362	61.163	1.00 39.27
		MOTA	3183	N	GLY A		27.670	21.921	59.826	
	15									1.00 22.02
	13	MOTA	3184	CA	GLY A		27.167	20.908	58.928	1.00 22.77
		ATOM	3185	С	GLY A		25.698	20.676	59.206	1.00 31.85
		MOTA	3186	0	GLY A	405	24.885	20.438	58.297	1.00 33.01
1		MOTA	3187	N	PHE A	406	25.364	20.747	60.493	1.00 26.28
		MOTA	3188	CA	PHE A	406	23.992	20.565	60.863	1.00 25.27
THE PARTY NAMED IN	20	ATOM	3189	C	PHE A		23.188	21.757	60.365	1.00 34.80
	20									
1		ATOM	3190	0	PHE A		22.195	21.629	59.638	1.00 36.22
3=4.		ATOM	3191	CB	PHE A		23.798	20.268	62.351	1.00 24.52
III.		ATOM	3192	CG	PHE A	406	22.388	20.525	62.798	1.00 24.82
E STOR		ATOM	3193	CD1	PHE A	406	21.328	19.734	62.353	1.00 28.50
(F)	25	ATOM	3194	CD2	PHE A	406	22.107	21.579	63.669	1.00 30.12
LT.		ATOM	3195		PHE A		20.025	19.977	62.793	
										1.00 31.40
		ATOM	3196		PHE A		20.810	21.862	64.105	1.00 32.57
123		ATOM	3197	CZ	PHE A		19.771	21.037	63.669	1.00 31.88
-4		ATOM	3198	N	LEU A	407	23.661	22.934	60.708	1.00 32.11
T.	30	ATOM	3199	CA	LEU A	407	22.972	24.132	60.269	1.00 33.11
		ATOM	3200	С	LEU A		22.706	24.204	58.767	1.00 34.74
M.		ATOM	3201	ō	LEU A		21.635	24.615	58.341	
										1.00 35.21
44 MC		MOTA	3202	CB	LEU A		23.589	25.420	60.840	1.00 35.36
54 H	-	ATOM	3203	CG	LEU A		22.597	26.577	60.855	1.00 41.79
A Ba	35	MOTA	3204	CD1	LEU A	407	23.048	27.626	61.833	1.00 40.45
		MOTA	3205	CD2	LEU A	407	22.513	27.197	59.461	1.00 49.57
		MOTA	3206	N	LYS A		23.667	23.804	57.948	1.00 34.92
		ATOM	3207	CA	LYS A		23.476	23.826	56.490	1.00 36.29
		ATOM	3208	C				22.876		
	40				LYS A		22.378		56.037	1.00 38.15
	40	ATOM	3209	0	LYS A		21.568	23.191	55.160	1.00 35.09
		ATOM	3210	CB	LYS A		24.747	23.517	55.707	1.00 40.54
		ATOM	3211	CG	LYS A	408	24.633	23.873	54.214	1.00 43.41
		MOTA	3212	CD	LYS A	408	25.950	23.796	53.422	1.00 49.26
		ATOM	3213	CE	LYS A		26.808	25.059	53.459	1.00 61.45
	45	ATOM	3214	NZ	LYS A		28.014	24.994	52.606	1.00 73.78
	•••	ATOM	3215							
				N	ALA A		22.352	21.690	56.655	1.00 35.34
		ATOM	3216	CA	ALA A		21.333	20.698	56.298	1.00 36.14
		ATOM	3217	С	ALA A	409	19.927	21.041	56.814	1.00 38.45
		MOTA	3218	0	ALA A	409	18.913	20.821	56.134	1.00 37.39
	50	ATOM	3219	CB	ALA A	409	21.762	19.273	56,626	1.00 36.66
		MOTA	3220	N	TYR A		19.902	21.597	58.030	1.00 33.14
		MOTA	3221	CA	TYR A		18.693	22.059	58.682	1.00 29.65
		MOTA	3222	C	TYR A		18.028	23.051	57.730	1.00 35.55
	e- e-	ATOM	3223	0	TYR A		16.855	22.976	57.399	1.00 37.26
	55	MOTA	3224	CB	TYR A	410	19.117	22.762	59 .9 70	1.00 24.67
		MOTA	3225	CG	TYR A	410	18.069	23.643	60.541	1.00 26.95
		ATOM	3226		TYR A		16.861	23.112	60.990	1.00 28.10
		ATOM	3227		TYR A		18.288	25.015	60.663	
										1.00 29.66
-	60	ATOM	3228		TYR A		15.883	23.924	61.571	1.00 26.98
	60	ATOM	3229		TYR A		17.316	25.839	61.230	1.00 31.84
		ATOM	3230	CZ	TYR A		16.112	25.294	61.685	1.00 37.49
		ATOM	3231	OH	TYR A	410	15.156	26.110	62.241	1.00 33.48
		ATOM	3232	N	VAL A		18.848	23.961	57.262	1.00 28.75
		ATOM	3233	CA	VAL A		18.457	24.984	56.341	1.00 29.23
			7.7			177		21.501	50.031	42.23

	ATOM	3234	С	VAL A	411	18.013	24.469	E4 000	1 00 04 00
								54.992	1.00 34.00
	ATOM	3235	0	VAL A		17.060	24.982	54.401	1.00 30.00
	MOTA	3236	CB	VAL A	411	19.617	25.922	56.139	1.00 32.22
	ATOM	3237	CGI	VAL A	411	19.331			
5							26.821	54.950	1.00 29.86
J .	MOTA	3238		VAL A		19.850	26.708	57.431	1.00 31.69
	ATOM	3239	N	GLU A	412	18.730	23.479	54.488	1.00 33.14
	MOTA	3240	CA	GLU A					
							22.900	53.217	1.00 31.91
	ATOM	3241	С	GLU A	412	17.068	22.163	53.355	1.00 30.32
	ATOM	3242	0	GLU A	412	16.182	22.225	52.531	1.00 31.89
10	ATOM	3243	CB	GLU A					
10						19.502	21.883	52.932	1.00 36.48
	ATOM	3244	CG	GLU A	412	20.443	22.174	51.737	1.00 67.01
	ATOM	3245	CD	GLU A	412	21.872	21.699	51.962	1.00100.00
	ATOM	3246		GLU A					
						22.193	20.782	52.716	1.00100.00
	ATOM	3247	OE2	GLU A	412	22.750	22.396	51.277	1.00 94.73
15	ATOM	3248	N	LYS A	413	16.922	21.444	54.444	
	ATOM	3249	CA						1.00 22.18
				LYS A		15.729	20.692	54.714	1.00 17.91
	ATOM	3250	С	LYS A	413	14.463	21.486	54.855	1.00 23.75
	ATOM	3251	0	LYS A	413	13.417	20.978		
								54.503	1.00 25.92
20	ATOM	3252	CB	LYS A		15.890	19.911	55.988	1.00 15.65
20	ATOM	3253	CG	LYS A	413	14.554	19.422	56.503	1.00 38.69
	ATOM	3254	CD	LYS A					
						14.150	18.089	55.903	1.00 58.11
	ATOM	3255	CE	LYS A	413	13.634	17.099	56.937	1.00 64.98
	ATOM	3256	NZ	LYS A	413	13.457	15.751	56.381	
	ATOM	3257	N						1.00 73.89
25				PHE A		14.530	22.688	55.424	1.00 25.40
23	MOTA	3258	CA	PHE A	414	13.316	23.479	55.640	1.00 27.80
	ATOM	3259	С	PHE A	414	13.151	24.748	54.821	
	ATOM	3260	O						1.00 35.82
				PHE A		12.276	25.557	55.122	1.00 35.17
	ATOM	3261	CB	PHE A	414	13.063	23.791	57.118	1.00 30.46
	ATOM	3262	CG	PHE A	414	12.936	22.553	57.964	
30	ATOM	3263		PHE A					1.00 33.88
50			CDI	FRE A	414	11.746	21.826	57.996	1.00 35.94
	ATOM	3264		PHE A		14.005	22.110	58.742	1.00 37.75
	ATOM	3265	CE1	PHE A	414	11.629	20.664	58.761	
	ATOM	3266							1.00 37.77
				PHE A		13.888	20.962	59.526	1.00 42.23
	ATOM	· 3267	CZ	PHE A	414	12.698	20.231	59.542	1.00 39.10
35	ATOM	3268	N	SER A	415	13.970	24.933		
	ATOM	3269	CA					53.795	1.00 36.12
				SER A		13.858	26.115	52.945	1.00 36.36
	ATOM	3270	С	SER A	415	12.412	26.295	52.510	1.00 38.99
	ATOM	3271	0	SER A	415	11.730	25.315	52.243	
	ATOM	3272	CB	SER A					1.00 41.04
40						14.773	26.008	51.736	1.00 37.43
40	MOTA	3273	OG	SER A	415	16.036	26.566	52.046	1.00 46.73
	ATOM	3274	N	TYR A	416	11.928	27.537	52.475	
	ATOM	3275	CA	TYR A					1.00 33.40
						10.541	27.832	52.072	1.00 30.88
	ATOM	3276	С	TYR A	416	9.453	27.183	52.947	1.00 33.62
	ATOM	3277	0	TYR A	416	8.295	27.095	52.546	
45	ATOM	3278		TYR A					1.00 33.44
							27.479	50.584	1.00 28.42
	MOTA	3279	CG	TYR A		11.496	27.782	49.723	1.00 24.76
	ATOM	3280	CD1	TYR A	416	11.791	29.087	49.338	1.00 26.55
	ATOM	3281		TYR A		12.375			
	ATOM		OPI	T11(1)	110		26.778	49.335	1.00 21.68
50		3282		TYR A		12.914	29.384	48.570	1.00 25.16
50	ATOM	3283	CE2	TYR A	416	13.504	27.052	48.572	1.00 20.15
	ATOM	3284	CZ	TYR A					
							28.360	48.189	1.00 30.62
	ATOM	3285		TYR A		14.892	28.616	47.399	1.00 35.15
	ATOM	3286	N	LYS A	417	9.823	26.713	54.122	1.00 27.67
	ATOM	3287		LYS A					
55							26.065	55.008	1.00 28.02
23	ATOM	3288	С	LYS A	417	8.733	26.830	56.317	1.00 31.36
	ATOM	3289	0	LYS A	417		27.671	56.682	
	ATOM	3290							1.00 33.15
				LYS A			24.615	55.252	1.00 33.86
	ATOM	3291	CG	LYS A	417	8.449	23.792	56.201	1.00 86.28
	ATOM	3292		LYS A			22.275	56.232	
60	ATOM	3293							1.00100.00
				LYS A			21.471	57.265	1.00 72.28
	ATOM	3294		LYS A		8.280	20.033	57.323	1.00 41.88
	MOTA	3295	N	SER A	418		26.557	57.033	
	ATOM	3296		SER A					1.00 28.88
							27.195	58.335	1.00 30.04
	ATOM	3297	C	SER A	418	7.425	26.064	59.332	1.00 34.09
						8			

		ATOM	3298	0	SER A	418	6.614	25.145	59.193	1 00	31.54
		ATOM	3299	СВ	SER A		6.261	28.126	58.410		31.46
		ATOM	3300	OG							
					SER A		6.417	29.106	57.399		35.01
	-	ATOM	3301	N	ILE A		8.356	26.077	60.281		28.50
	5	ATOM	3302	CA	ILE A		8.446	24.971	61.205		23.86
		MOTA	3303	С	ILE A		8.272	25.342	62.641	1.00	25.06
		MOTA	3304	0	ILE A	419	8.122	26.500	63.002	1.00	21.64
		MOTA	3305	CB	ILE A	419	9.803	24.314	61.026	1.00	25.02
		MOTA	3306	CG1	ILE A	419	10.863	25.325	61.399		23.63
	10	ATOM	3307		ILE A		10.051	23.937	59.565		23.22
	10	ATOM	3308		ILE A		12.236	24.688	61.253		23.48
			3309		THR A						
		ATOM		N			8.321	24.302	63.455		24.71
		ATOM	3310	CA	THR A		8.201	24.417	64.895		24.36
		ATOM	3311	С	THR A		9.416	23.795	65.538		28.90
	15	MOTA	3312	0	THR A		10.190	23.112	64.863	1.00	23.38
		ATOM	3313	CB	THR A	420	6.979	23.691	65.448	1.00	24.92
		MOTA	3314	OG1	THR A	420	7.190	22.313	65.291	1.00	26.43
		MOTA	3315		THR A		5.728	24.082	64.694		31.57
and the		MOTA	3316	N	THR A		9.542	24.051	66.855		29.30
100	20	ATOM	3317	CA	THR A		10.610	23.549	67.709		
£4 ##¢	20		3318	C	THR A						27.78
43		ATOM					10.831	22.035	67.585		30.99
i.4.		ATOM	3319	0	THR A		11.975	21.594	67.489	1.00	33.28
		ATOM	3320	CB	THR A		10.394	23.969	69.166	1.00	21.94
Higher Test		ATOM	3321	OG1	THR A	421	10.567	25.369	69.263	1.00	24.52
संबंधार इसके	25	MOTA	3322	CG2	THR A	421	11.399	23.221	70.045		20.12
		MOTA	3323	N	ASP A		9.721	21.272	67.575		21.94
. 1997 PA		ATOM	3324	CA	ASP A		9.706	19.823	67.430		
i i		ATOM	3325	C	ASP A						21.08
· 107							10.323	19.401	66.104		31.16
g=40	30	ATOM	3326	0_	ASP A		11.110	18.427	66.027		31.95
# D	30	ATOM	3327	СВ	ASP A		8.276	19.278	67.561		19.49
12 (125) 1925 - 35		ATOM	3328	CG	ASP A		8.236	17.802	67.298	1.00	31.85
		ATOM	3329	ODl	ASP A	422	9.130	17.040	67.654	1.00	29.73
49		ATOM	3330	OD2	ASP A	422	7.197	17.415	66.598	1.00	56.60
140		ATOM	3331	N	ASP A	423	9.957	20.146	65.049		26.75
35.00	35	MOTA	3332	CA	ASP A		10.505	19.876	63.729		26.01
in the	-	ATOM	3333	C	ASP A		12.027	19.957	63.830		40.09
		MOTA	3334	Õ	ASP A		12.753				
		ATOM	3335	CB	ASP A			19.020	63.500		47.09
							10.000	20.833	62.631		24.86
	40	ATOM	3336	CG	ASP A		8.538	20.722	62.343		39.90
	40	ATOM	3337		ASP A		7.968	19.649	62.299	1.00	45.03
		ATOM	3338	OD2	ASP A		7.943	21.887	62.113	1.00	40.43
		ATOM	3339	N	TRP A	424	12.493	21.099	64.320	1.00	31.92
		ATOM	3340	CA	TRP A	424	13.903	21.372	64.495	1.00	29.69
		ATOM	3341	С	TRP A	424	14.611	20.271	65.282		33.81
	45	MOTA	3342	0	TRP A	424	15.537	19.616	64.824		35.87
		MOTA	3343	CB	TRP A		14.056	22.711	65.239		26.11
		ATOM	3344	CG	TRP A		15.431	22.869	65.786		
		ATOM	3345								27.05
					TRP A		16.518	23.302	65.101		29.65
	50	ATOM	3346		TRP A		15.885	22.587	67.119		26.62
	50	MOTA	3347		TRP A		17.612	23.321	65.922		27.83
		ATOM	3348		TRP A		17.257	22.891	67.163	1.00	28.62
		ATOM	3349		TRP A		15.260	22.138	68.269	1.00	29.69
		ATOM	3350	CZ2	TRP A	424	18.010	22.758	68.319		29.28
		MOTA	3351		TRP A		16.000	21.993	69.429		33.50
	55	MOTA	3352		TRP A		17.362	22.317	69.459		33.93
		ATOM	3353	N	LYS A		14.156	20.090	66.497		
		ATOM	3354	CA							28.75
					LYS A		14.723	19.105	67.373		29.43
		ATOM	3355	C	LYS A		14.697	17.691	66.808		29.49
	<i>د</i> م	ATOM	3356	0	LYS A		15.627	16.928	67.030	1.00	27.65
	60	MOTA	3357	CB	LYS A		14.078	19.171	68.744	1.00	29.70
		ATOM	3358	CG	LYS A	425	14.860	18.414	69.787		28.11
		ATOM	3359	CD	LYS A		14.161	18.409	71.132		23.57
		MOTA	3360	CE	LYS A		14.300	17.063	71.815		36.16
		MOTA	3361	NZ	LYS A		13.042	16.302	71.768		58.08
										_ ,	~~~~

	ATOM	3362	N	ASP A 4	126	13.606	17.361	66.107	1.00 19.05
	ATOM	3363	CA	ASP A 4		13.417	16.070	65.516	1.00 19.03
	ATOM	3364	C	ASP A 4					
						14.453	15.879	64.387	1.00 28.33
<u>.</u>	ATOM	3365	0	ASP A 4		15.070	14.832	64.232	1.00 31.25
5	ATOM	3366	CB	ASP A 4		11.920	15.840	65.098	1.00 19.79
	ATOM	3367	CG	ASP A 4	126	10.998	15.575	66.274	1.00 25.54
	ATOM	3368	OD1	ASP A 4	126 ·	11.341	15,466	67.409	1.00 29.73
	MOTA	3369		ASP A 4		9.804	15.611	65.938	1.00 20.67
	ATOM	3370	N	PHE A 4		14.674	16.926	63.612	
10									1.00 25.09
10	ATOM	3371	CA	PHE A 4		15.654	16.899	62.540	1.00 25.81
	ATOM	3372	С	PHE A 4		17.066	16.718	63.159	1.00 34.01
	MOTA	3373	0	PHE A 4	127	17.843	15.851	62.773	1.00 36.25
	MOTA	3374	CB	PHE A 4	127	15.589	18.197	61.704	1.00 26.35
	ATOM	3375	CG	PHE A 4	127	16.698	18.202	60.702	1.00 27.40
15	MOTA	3376	CD1	PHE A 4		16.714	17.247	59.686	1.00 29.97
	ATOM	3377		PHE A 4		17.773	19.084	60.805	
		3378		PHE A 4					1.00 28.71
	ATOM					17.730	17.194	58.733	1.00 27.72
	ATOM	3379	CE2	PHE A 4		18.806	19.046	59.867	1.00 30.37
	MOTA	3380	CZ	PHE A 4	127	18.780	18.104	58.837	1.00 26.34
20	MOTA	3381	N	LEU A 4	128	17.369	17.544	64.160	1.00 28.94
	MOTA	3382	CA	LEU A 4	128	18.622	17.496	64.924	1.00 27.74
* * .	ATOM	3383	С	LEU A 4		18.989	16.047	65.303	1.00 32.08
	ATOM	3384	ŏ	LEU A 4		20.145			
							15.647	65.209	1.00 36.38
25	ATOM	3385	CB	LEU A 4		18.510	18.362	66.223	1.00 24.68
25	ATOM	3386	CG	LEU A 4		19.778	18.377	67.079	1.00 24.30
	MOTA	3387	CD1			20.855	19.278	66.467	1.00 23.00
	ATOM	3388	CD2	LEU A 4	128	19.446	18.856	68.481	1.00 16.41
	ATOM	3389	N	TYR A 4		17.991	15.271	65.735	1.00 23.71
	ATOM	3390	CA	TYR A 4		18.148	13.896	66.144	1.00 23.18
30	ATOM	3391	C	TYR A 4					
50						18.311	12.967	64.976	1.00 26.62
	ATOM	3392	0	TYR A 4		18.911	11.910	65.076	1.00 28.43
	ATOM	3393	CB	TYR A 4		16.921	13.453	66.914	1.00 25.59
	ATOM	3394	CG	TYR A 4		17.069	13.526	68.414	1.00 29.53
	MOTA	3395	CD1	TYR A 4	129	16.823	14.714	69.114	1.00 31.11
35	ATOM	3396	CD2	TYR A 4	129	17.361	12.383	69.156	1.00 32.70
	ATOM	3397	CE1	TYR A 4		16.916	14.769	70.510	1.00 32.23
	ATOM	3398	CE2	TYR A 4		17.485	12.420	70.551	
	ATOM	3399	CZ	TYR À 4					1.00 35.30
						17.251	13.623	71.231	1.00 41.02
40	MOTA	3400	OH	TYR A 4		17.339	13.679	72.609	1.00 30.02
40	ATOM	3401	N	SER A 4		17.748	13.342	63.854	1.00 21.68
	ATOM	3402	CA	SER A 4	130	17.914	12.469	62.730	1.00 23.42
	MOTA	3403	С	SER A 4	130	19.264	12.722	62.050	1.00 32.87
	ATOM	3404	0	SER A 4	130	19.879	11.819	61.467	1.00 35.11
	ATOM	3405	CB	SER A 4	130	16.756	12.541	61.773	1.00 28.79
45	ATOM	3406	OG	SER A 4		17.089	13.475	60.777	1.00 20.75
	ATOM	3407	N	TYR A 4					
						19.748	13.955	62.132	1.00 27.18
	ATOM	3408	CA	TYR A 4		21.017	14.296	61.537	1.00 27.14
	MOTA	3409	С	TYR A 4		22.152	13.702	62.316	1.00 32.52
50	ATOM	3410	0	TYR A 4		23.155	13.242	61.771	1.00 33.64
50	ATOM	3411	CB	TYR A 4	131	21.216	15.818	61.385	1.00 31.07
	ATOM	3412	CG	TYR A 4	131	22.566	16.265	60.812	1.00 35.63
	ATOM	3413		TYR A 4		23.663	16.492	61.650	1.00 36.88
	ATOM	3414		TYR A 4		22.735	16.496		
	ATOM	3415		TYR A 4				59.444	1.00 36.92
55						24.894	16.924	61.157	1.00 33.78
23	ATOM	3416	CE2	TYR A 4		23.964	16.916	58.924	1.00 37.86
	MOTA	3417	CZ	TYR A 4		25.038	17.143	59.786	1.00 46.01
	ATOM	3418	OH	TYR A 4	131	26.247	17.573	59.294	1.00 51.28
	ATOM	3419	N	PHE A 4	132	21.964	13.728	63.606	1.00 29.66
	ATOM	3420	CA	PHE A 4		22.939	13.215	64.526	1.00 29.12
60	ATOM	3421	C	PHE A 4		22.522	11.865	65.007	1.00 23.12
	ATOM	3422	Ö	PHE A 4					
	ATOM	3423	СВ			22.499	11.593	66.197	1.00 46.77
				PHE A 4		23.063	14.157	65.719	1.00 30.24
	ATOM	3424	CG	PHE A 4		23.962	15.327	65.401	1.00 33.03
	MOTA	3425	CDI	PHE A 4	132	25.336	15.113	65.277	1.00 37.22

	MOTA	3426		PHE A		23.470	16.624	65.232	1.00 30.70
	MOTA	3427		PHE A		26.223	16.153	64.999	1.00 34.27
	ATOM	3428		PHE A		24.349	17.667	64.938	1.00 31.71
_	ATOM	3429	CZ	PHE A		25.722	17.438	64.823	1.00 27.82
5	ATOM	3430	N	LYS A		22.174	11.029	64.063	1.00 42.50
	ATOM	3431	CA	LYS A		21.669	9.670	64.270	1.00 40.87
	ATOM	3432	С	LYS A		22.718	8.751	64.908	1.00 46.17
	ATOM	3433	0	LYS A		22.405	7.734	65.513	1.00 48.48
	MOTA	3434	CB	LYS A		21.245	9.106	62.917	1.00 39.25
10	ATOM	3435	CG	LYS A		19.988	8.241	63.017	1.00 84.17
	MOTA	3436	CD	LYS A		18.925	8.660	62.000	1.00100.00
	MOTA	3437	CE	LYS A	433	17.523	8.172	62.384	1.00100.00
	MOTA	3438	NZ	LYS A	433	16.525	9.119	61.884	1.00100.00
* *	MOTA	3439	N	ASP A		24.002	9.112	64.697	1.00 45.20
15	MOTA	3440	CA	ASP A		25.083	8.349	65.321	1.00 47.80
	MOTA	3441	С	ASP A		25.201	8.684	66.802	1.00 50.78
	MOTA	3442	0	ASP A		25.474	7.845	67.653	1.00 55.76
. C 10.	ATOM	3443	CB	ASP A		26.405	8.567	64.562	1.00 53.91
G	ATOM	3444	CG	ASP A		26.123	8.474	63.069	1.00 93.32
20	ATOM	3445		ASP A		25.744	7.573	62.325	1.00 96.22
200	MOTA	3446	OD2	ASP A		26.119	9.664	62.753	1.00100.00
ge Si.	ATOM	3447	N	LYS A		25.015	9.978	67.085	1.00 38.82
170	MOTA	3448	CA	LYS A	435	24.974	10.404	68.468	1.00 34.57
25	ATOM	3449	С	LYS A	435	23.549	10.749	68.881	1.00 39.87
25	MOTA	3450	0	LYS A	435	23.070	11.840	68.693	1.00 40.34
	MOTA	3451	CB	LYS A		25.864	11.631	68.615	1.00 34.69
1-4-	ATOM	3452	CG	LYS A		27.064	11.595	67.679	1.00 40.86
麗 -	ATOM	3453	CD	LYS A		27.703	12.975	67.532	1.00 51.04
}-A-	ATOM	3454	CE	LYS A	435	29.242	12.904	67.557	1.00 24.08
30	ATOM	3455	NZ	LYS A		29.822	13.990	66.760	1.00 45.26
	ATOM	3456	N	VAL A		22.843	9.728	69.414	1.00 38.07
त्रे व्यक्ति सम्बद्धाः	MOTA	3457	CA	VAL A		21.601	10.036	70.111	1.00 36.86
14 m) 14 m)	MOTA	3458	С	VAL A		21.846	10.129	71.608	1.00 44.88
	MOTA	3459	0	VAL A		21.289	10.948	72.300	1.00 46.42
4435	MOTA	3460	CB	VAL A		20.567	8.923	69.816	1.00 37.37
	MOTA	3461		VAL A		19.944	9.143	68.446	1.00 36.24
	ATOM	3462		VAL A		21.227	7.556	69.854	1.00 36.80
	ATOM	3463	N	ASP A		22.718	9.232	72.099	1.00 43.61
40	ATOM	3464	CA	ASP A		23.044	9.222	73.522	1.00 41.43
40	ATOM	3465	C	ASP A		23.657	10.546	73.958	1.00 45.71
	ATOM	3466	0	ASP A		23.554	10.956	75.107	1.00 49.89
	ATOM	3467	CB	ASP A		24.022	8.082	73.776	1.00 43.84
	ATOM	3468	CG	ASP A		23.281	6.752	73.691	1.00 72.47
45	ATOM	3469		ASP A		22.062	6.769	73.823	1.00 74.64
45	ATOM	3470		ASP A		23.933	5.730	73.481	1.00 86.09
	ATOM	3471	N	VAL A		24.333	11.324	73.122	1.00 40.21
	ATOM	3472	CA	VAL A		24.807		73.577	1.00 40.97
	ATOM	3473	C	VAL A		23.621	13.582	73.668	1.00 41.86
50	ATOM	3474	0	VAL A		23.368	14.276	74.657	1.00 39.95
30	ATOM	3475	CB	VAL A		25.875	13.165	72.615	1.00 47.47
	ATOM	3476		VAL A		26.438	14.523	73.051	1.00 47.51
	ATOM	3477		VAL A		26.996	12.149	72.440	1.00 47.51
	MOTA MOTA	3478 3479	N CA	LEU A		22.876 21.729	13.595 14.442	72.585 72.507	1.00 37.91
55	ATOM	3479	C						1.00 36.21
	ATOM	3481	0	LEU A		20.850 20.214	14.190 15.064	73.695	1.00 40.03
	ATOM	3482	CB	LEU A				74.255	1.00 42.22
	ATOM	3483	CG	LEU A		20.949	14.180	71.210	1.00 33.84
				LEU A		21.552	14.939	70.039	1.00 32.80
60	ATOM ATOM	3484 3485		LEU A		20.813	14.538	68.775	1.00 34.08
00	ATOM	3486	N	ASN A		21.435 20.810	16.434 12.953	70.258 74.076	1.00 23.80
	ATOM	3487		ASN A		19.971	12.933	75.187	1.00 34.03 1.00 34.00
	ATOM	3488	CA	ASN A		20.494	13.093	76.532	1.00 34.00
	ATOM	3489	0			19.816		77.544	
	ALOM	2403	9	ASN A	440	13.010	12.995	11.044	1.00 42.09

	ATOM	3490	CP	TACKE TA	440	10 601				
			CB	ASN A		19.681	11.095	75.178	1.00	24.89
	MOTA	3491	CG	ASN A		18.790	10.635	74.028		46.52
	ATOM	3492	OD1	ASN A	440	19.005	9.537	73.480		58.82
	ATOM	3493		ASN A		17.769				
5	ATOM	3494					11.440	73.680		31.11
			N	GLN A		21.707	13.623	76.531	1.00	36.98
	ATOM	3495	CA	GLN A		22.339	14.095	77.744		35.47
	ATOM	3496	C	GLN A	441	21.879	15.478	78.067		36.00
	ATOM	3497	0	GLN A		22.137				
							16.029	79.142		34.96
10	ATOM	3498	CB	GLN A		23.878	14.109	77.581	1.00	38.10
10	ATOM	3499	CG	GLN A	441	24.504	12.692	77.422		52.06
	ATOM	3500	CD	GLN A	441	25.954	12.730	76.955		
	ATOM	3501	OE1	GLN A						81.69
						26.476	13.796	76.609		74.46
	ATOM	3502	NE2	GLN A		26.616	11.574	76.972	1.00	91.09
	ATOM	3503	N	VAL A	442	21.197	16.067	77.112		31.86
15	ATOM	3504	CA	VAL A		20.753	17.411	77.384		
	ATOM	3505	С							32.78
				VAL A		19.354	17.468	77.970	1.00	38.24
	MOTA	3506	0	VAL A	442	18.468	16.700	77.588	1.00	42.83
	MOTA	3507	CB	VAL A	442	20.845	18.277	76.159		34.84
	ATOM	3508	CG1			21.430	17.435			
20	ATOM	3509						75.020	1.00	34.65
20				VAL A		19.441	18.705	75.811	1.00	33.21
	MOTA	3510	N	ASP A	443	19.172	18.388	78.908		25.60
	ATOM	3511	CA	ASP A	443	17.931	18.634	79.616		
	MOTA	3512	С	ASP A		16.996		75.010		24.57
	ATOM						19.533	78.791	1.00	32.14
25		3513	0	ASP A		16.744	20.732	79.073	1.00	34.77
25	ATOM	3514	СВ	ASP A		18.332	19.272	80.957		27.11
	ATOM	3515	CG	ASP A	443	17.216	19.413	81.901		39.99
	ATOM	3516	OD1	ASP A	443					
	ATOM	3517				16.063	19.234	81.573		44.78
				ASP A		17.631	19.753	83.094	1.00	56.66
-00	ATOM	3518	N	TRP A		16.525	18.914	77.722		28.30
30	ATOM	3519	CA	TRP A	444	15.614	19.507	76.757	1 00	26.27
	ATOM	3520	С	TRP A		14.460			1.00	20.27
	ATOM	3521					20.296	77.416		31.52
			0	TRP A		14.102	21.409	76.988	1.00	34.63
	ATOM	3522	CB	TRP A		15.067	18.398	75.799	1.00	21.47
	MOTA	3523	CG	TRP A	444	16.095	17.951	74.806		22.03
35	ATOM	3524	CD1	TRP A		16.675				
	ATOM	3525	CD2				16.718	74.736		25.16
				TRP A		16.733	18.738	73.776	1.00	20.36
	MOTA	3526		TRP A		17.623	16.677	73.738		23.97
	ATOM	3527	CE2	TRP A	444	17.688	17.906	73.138		24.71
	ATOM	3528		TRP A		16.596				
40	MOTA	3529					20.045	73.342		20.86
				TRP A		18.448	18.345	72.060	1.00	24.51
	MOTA	3530		TRP A		17.353	20.471	72.264	1.00	22.88
	MOTA	3531	CH2	TRP A	444	18.281	19.643	71.643		23.48
	MOTA	3532	N	ASN A		13.855	19.711			
	ATOM	3533	CA	ASN A				78.457		24.92
45				-		12.723	20.326	79.113	1.00	26.30
73	ATOM	3534		ASN A		13.040	21.677	79.729	1.00	30.17
	MOTA	3535	0	ASN A	445	12.291	22.660	79.547		31.86
	ATOM	3536	CB	ASN A	445	11.987	19.382	80.094		
	MOTA	3537		ASN A				00.094		40.83
	ATOM	3538	001	ACM A	445	10.946	20.033	81.020		87.07
50				ASN A		11.271	20.635	82.065	1.00	86.38
<i>3</i> 0	ATOM	3539	ND2	ASN A	445	9.670	19.848	80.688		71.65
	MOTA	3540	N	ALA A	446	14.147	21.687	80.436		
	ATOM	3541	CA	ALA A	446	14.583				22.70
	MOTA	3542					22.886	81.073		24.45
				ALA A		14.886	23.896	79.990	1.00	30.52
	ATOM	3543	0	ALA A	446	14.324	25.001	79.936		33.92
55	ATOM	3544		ALA A		15.814	22.543	81.900		
	ATOM	3545								25.68
				TRP A		15.776	23.494	79.102		25.24
	ATOM	3546		TRP A		16.162	24.384	78.034		26.83
	ATOM	3547	С	TRP A	447	14.989	24.912	77.223		31.32
	ATOM	3548		TRP A		14.971	26.089			
60	ATOM	3549		TRP A				76.875		30.48
						17.166	23.725	77.062		25.78
	ATOM	3550		TRP A		18.625	23.815	77.421		26.60
	ATOM	3551	CD1	TRP A	447	19.343	22.840	78.046		28.89
	MOTA	3552		TRP A		19.554	24.896	77.165	1 00	26 16
	ATOM -	3553		TRP A					T.00	26.16
				***** 'L'	171	20.654	23.217	78.197	T.00	27.23

	ATOM	3554	CE2	TRP A 447	20.822	24.476	77.660	1.00 29.00
	ATOM	3555		TRP A 447	19.435	26.162	76.607	1.00 27.56
	ATOM	3556	CZ2		21.954	25.290	77.583	1.00 27.95
	ATOM	3557	CZ3	TRP A 447	20.554	26.966	76.538	1.00 29.93
5	ATOM	3558	CH2	TRP A 447	21.792	26.539	77.035	1.00 20.16
,	MOTA	3559	N	LEU A 448	14.029	24.034	76.893	1.00 36.10
	ATOM	3560	CA	LEU A 448	12.896	24.421	76.052	1.00 26.92
		3561	C	LEU A 448	11.734	25.064	76.779	
	ATOM			LEU A 448				1.00 36.15
10	ATOM	3562	O		11.089	26.031	76.304	1.00 31.19
10	ATOM	3563	CB	LEU A 448	12.338	23.197	75.307	1.00 25.26
	ATOM	3564	CG	LEU A 448	13.311	22.545	74.332	1.00 28.29
	ATOM	3565		LEU A 448	12.597	21.455	73.530	1.00 30.49
	ATOM	3566		LEU A 448	13.879	23.576	73.375	1.00 21.94
	MOTA	3567	N	TYR A 449	11.472	24.455	77.924	1.00 33.14
15	MOTA	3568	CA	TYR A 449	10.373	24.835	78.747	1.00 30.64
	ATOM	3569	С	TYR A 449	10.646	25.525	80.041	1.00 34.31
	MOTA	3570	0	TYR A 449	9 .7 50	26.191	80.529	1.00 41.98
	MOTA	3571	CB	TYR A 449	9.400	23.674	78.916	1.00 29.14
	MOTA	3572	CG	TYR A 449	9.212	23.089	77.556	1.00 26.50
20	ATOM	3573	CD1	TYR A 449	8.762	23.869	76.485	1.00 24.36
	MOTA	3574	CD2	TYR A 449	9.560	21.762	77.325	1.00 28.48
	MOTA	3575		TYR A 449	8.626	23.331	75.202	1.00 17.56
	ATOM	3576	CE2	TYR A 449	9.427	21.205	76.054	1.00 29.93
	ATOM	3577	CZ	TYR A 449	8.959	21.988	74.998	1.00 23.55
25	MOTA	3578	OH	TYR A 449	8.840	21.415	73.762	1.00 39.47
20	MOTA	3579	N	SER A 450	11.806	25.413	80.644	1.00 33.47
	ATOM	3580	CA	SER A 450	11.902	26.149		
		3581	C	SER A 450	12.278		81.900	1.00 21.21
	MOTA					27.625	81.749	1.00 23.98
30	ATOM	3582	0	SER A 450	12.966	28.035	80.810	1.00 27.17
30	ATOM	3583	CB	SER A 450	12.666	25.436	83.010	1.00 24.83
	ATOM	3584	OG	SER A 450	12.540	24.046	82.871	1.00 36.29
	ATOM	3585	N	PRO A 451	11.806	28.430	82.689	1.00 19.76
	MOTA	35,86	CA	PRO A 451	12.111	29.840	82.669	1.00 18.20
25	ATOM	3587	С	PRO A 451	13.461	29.988	83.271	1.00 21.72
35	ATOM	3588	0	PRO A 451	14.022	29.015	83.742	1.00 24.34
	MOTA	3589	CB	PRO A 451	11.185	30.485	83.695	1.00 18.85
	ATOM	3590	CG	PRO A 451	10.836	29.390	84.677	1.00 23.13
	ATOM	3591	CD	PRO A 451	11.002	28.078	83.900	1.00 19.61
4.0	ATOM	3592	N	GLY A 452	13.959	31.212	83.307	1.00 18.97
40	ATOM	3593	CA	GLY A 452	15.241	31.444	83.922	1.00 19.09
	ATOM	3594	С	GLY A 452	16.382	31.107	83.016	1.00 26.20
	MOTA	3595	0	GLY A 452	16.191	30.916	81.819	1.00 27.37
	ATOM	3596	N	LEU A 453	17.557	31.057	83.650	1.00 25.48
	MOTA	3597	CA	LEU A 453	18.843	30.750	83.029	1.00 25.32
45	ATOM	3598	С	LEU A 453	18.906	29.322	82.629	1.00 26.21
	ATOM	3599	0	LEU A 453	18.400	28.458	83.322	1.00 25.04
	MOTA	3600	CB	LEU A 453	20.042	31.119	83.938	1.00 25.46
	ATOM	3601	CG	LEU A 453	20.280	32.632	83.904	1.00 31.82
	ATOM	3602	CD1	LEU A 453	21.019	33.087	85.119	1.00 31.78
50	ATOM	3603		LEU A 453	21.046	33.056	82.651	1.00 41.50
	MOTA	3604	N	PRO A 454	19.510	29.082	81.489	1.00 22.97
	MOTA	3605	CA	PRO A 454	19.585	27.747	81.003	1.00 21.60
	ATOM	3606	C	PRO A 454	20,145	26.890	82.075	1.00 26.94
	MOTA	3607	Ö	PRO A 454	20.143	27.359	82.893	1.00 20.94
55	ATOM	3608	СВ	PRO A 454	20.489	27.780	79.768	1.00 22.34
	ATOM	3609	CG	PRO A 454	20.777	29.232	79.470	1.00 22.34
		3610	CD	PRO A 454				
	ATOM	3611	N	PRO A 454	20.136	30.054	80.556	1.00 20.82
	ATOM				19.721	25.648	82.067	1.00 25.61
60	MOTA	3612	CA	PRO A 455	20.167	24.683	83.031	1.00 24.27
UU	ATOM	3613	C	PRO A 455	21.661	24.568	82.991	1.00 30.95
	ATOM	3614	0	PRO A 455	22.225	24.062	83.920	1.00 33.47
	ATOM	3615	CB	PRO A 455	19.631	23.320	82.592	1.00 25.04
	ATOM	3616	CG	PRO A 455	19.149	23.497	81.162	1.00 33.02
	MOTA	3617	CD	PRO A 455	19.111	25.005	80.888	1.00 28.49

	MOTA	3618	N	ILE A	456	22.305	25.002	81.911	1.00 27.91
	ATOM	3619	CA	ILE A		23.764	24.893	81.821	1.00 27.82
	ATOM	3620	С	ILE A		24.395	26.057	81.077	1.00 27.82
	ATOM	3621	0	ILE A		23.737	26.769	80.293	1.00 34.73
5	ATOM	3622	CB	ILE A		24.228	23.540	81.259	1.00 37.01
	ATOM	3623	CG1			25.721	23.305	81.417	
	ATOM	3624	CG2			23.865	23.369	79.788	1.00 29.78
	ATOM	3625	CD1			26.054	21.852		1.00 32.96
	ATOM	3626	N	LYS A		25.680		81.116	1.00 23.94
10	ATOM	3627	CA	LYS A		26.405	26.252	81.334	1.00 30.52
10	ATOM	3628	c	LYS A			27.335	80.707	1.00 30.21
	ATOM	3629	õ	LYS A		27.515	26.808	79.835	1.00 32.14
	ATOM	3630	СВ			28.328	26.037	80.273	1.00 33.07
	ATOM	3631		LYS A		26.953	28.264	81.749	1.00 32.38
15	ATOM	3632	CG	LYS A		27.818	29.327	81.121	1.00 34.64
13			CD	LYS A		28.288	30.306	82.166	1.00 13.41
	ATOM	3633	CE	LYS A		28.803	31.596	81.565	1.00 18.04
	ATOM	3634	NZ	LYS A		28.974	32.643	82.595	1.00 26.77
	ATOM	3635	N	PRO A		27.567	27.208	78.589	1.00 27.50
20	ATOM	3636	CA	PRO A		28.630	26.675	77.737	1.00 26.85
20	ATOM	3637	С	PRO A		29.994	27.147	78.185	1.00 26.89
3	ATOM	3638	0	PRO A	458	30.128	27.876	79.167	1.00 24.86
	ATOM	3639	CB	PRO A	458	28.335	27.191	76.316	1.00 29.41
	ATOM	3640	CG	PRO A	458	26.952	27.864	76.375	1.00 33.24
	ATOM	3641	CD	PRO A	458	26.574	28.044	77.848	1.00 26.12
25	ATOM	3642	N	ASN A		31.005	26.754	77.440	1.00 20.12
	ATOM	3643	CA	ASN A		32.359	27.191	77.735	
	ATOM	3644	С	ASN A		32.751	28.325	76.820	1.00 22.29
	ATOM	3645	Ö	ASN A		32.451	28.296	75.617	1.00 30.27
	ATOM	3646	CB	ASN A		33.315	26.060	77.494	1.00 32.89
30	ATOM	3647	CG	ASN A		32.766	24.846		1.00 25.03
1	ATOM	3648		ASN A		32.700	24.822	78.155	1.00 49.54
	ATOM	3649	ND2	ASN A	450	32.411		79.383	1.00 50.09
	ATOM	3650	N	TYR A			23.870	77.332	1.00 38.39
	ATOM	3651	CA	TYR A		33.448	29.316	77.380	1.00 25.58
35	ATOM	3652	C	TYR A		33.851	30.493	76.625	1.00 23.89
	ATOM	3653	õ			35.298	30.853	76.745	1.00 34.20
	ATOM	3654	СВ	TYR A		35.849	30.862	77.839	1.00 35.27
	ATOM	3655	CG	TYR A		33.120	31.708	77.171	1.00 24.38
	ATOM	3656	CD1	TYR A		31.636	31.631	77.024	1.00 26.98
40	ATOM	3657				31.029	32.011	75.829	1.00 30.69
40			CD2	TYR A		30.838	31.168	78.064	1.00 25.70
	ATOM	3658	CE1	TYR A		29.644	31.952	75.684	1.00 28.77
	ATOM	3659	CE2	TYR A		29.453	31.096	77.938	1.00 25.24
	ATOM	3660	CZ	TYR A		28.863	31.496	76.741	1.00 24.49
45	ATOM	3661	OH	TYR A		27.519	31.443	76.587	1.00 28.39
43	ATOM	3662	N	ASP A		35.893	31.227	75.616	1.00 30.58
	ATOM	3663	CA	ASP A		37.268	31.640	75.654	1.00 27.51
	ATOM	3664	С	ASP A		37.319	32.941	76.464	1.00 23.53
	ATOM	3665	0	ASP A		36.377	33.704	76.396	1.00 26.62
· 60:	ATOM	3666	CB	ASP A	461	37.821	31.784	74.218	1.00 27.30
50	ATOM	3667	CG	ASP A	461	39.137	32.466	74.260	1.00 32.53
	ATOM	3668	OD1	ASP A	461	39.262	33.672	74.334	1.00 39.66
	ATOM	3669	OD2	ASP A	461	40.130	31.628	74.306	1.00 44.34
	ATOM	3670	N	MET A	462	38,375	33.234	77.224	1.00 17.26
	ATOM	3671	CA	MET A		38.396	34.511	78.008	1.00 18.66
55	ATOM	3672	С	MET A		39.299	35.634	77.485	1.00 24.02
	ATOM	3673	0	MET A		39.336	36.738	78.011	
	ATOM	3674	СВ	MET A		38.818	34.186	79.431	1.00 24.56
	ATOM	3675	CG	MET A		37.808	33.209	80.025	1.00 22.99
	ATOM	3676	SD	MET A		36.166	33.969		1.00 28.98
60	ATOM	3677	CE	MET A		36.420		79.951	1.00 33.22
	ATOM	3678	N	THR A			35.300	81.153	1.00 27.89
	ATOM	3679	CA	THR A		40.067	35.348	76.461	1.00 22.57
	ATOM	3680	C	THR A		41.015	36.285	75.911	1.00 22.64
	ATOM					40.690	37.738	75.961	1.00 33.12
	AL ON	3681	0	THR A	403	41.372	38.493	76.640	1.00 35.27

		ATOM	3682	СВ	THR A	163		41.574	35.929	74 506	1 00 00 00
		ATOM			THR A			41.939		74.536	1.00 29.80
		ATOM	3684		THR A			42.797	34.576 36.793	74.509	1.00 26.74
		ATOM	3685	N	LEU A					74.224	1.00 18.79
	5	ATOM	3686	CA	LEU A			39.700	38.141	75.177	1.00 30.50
	5							39.293	39.533	75.061	1.00 29.15
		ATOM	3687	C	LEU A			38.490	40.067	76.216	1.00 34.24
		ATOM	3688	0	LEU A		•	38.439	41.270	76.422	1.00 37.12
		ATOM		CB	LEU A			38.537	39.767	73.743	1.00 29.20
	10	MOTA	3690	CG	LEU A			39.393	39.394	72.527	1.00 33.73
	10	MOTA	3691		LEU A			38.609	39.565	71.217	1.00 32.72
		MOTA	3692	CD2	LEU A			40.648	40.261	72.499	1.00 26.22
		ATOM	3693	N	THR A	465		37.855	39.167	76.964	1.00 30.71
		ATOM	3694	CA	THR A	465		37.005	39.496	78.103	1.00 28.58
		MOTA	3695	С	THR A	465		37.800	39.893	79.324	1.00 30.69
	15	ATOM	3696	0	THR A			37.530	40.865	80.030	1.00 30.03
		ATOM	3697	СВ	THR A			36.016	38.328	78.372	1.00 31.27
		ATOM	3698		THR A			35.101	38.212		
.co eu.		ATOM	3699		THR A			35.255		77.296	1.00 50.93
		ATOM	3700	N	ASN A				38.451	79.690	1.00 26.34
100	20	ATOM	3701	CA				38.802	39.111	79.568	1.00 24.40
12	20				ASN A			39.635	39.375	80.688	1.00 23.11
L.A.		ATOM	3702	C	ASN A			39.899	40.856	80.967	1.00 28.37
E MOST		ATOM	3703	0	ASN A			39.763	41.270	82.120	1.00 27.03
		ATOM	3704	CB	ASN A			40.921	38.543	80.629	1.00 20.30
11 m	0.5	ATOM	3705	CG	ASN A			40.709	37.145	81.155	1.00 32.26
	25	MOTA	3706		ASN A			41.384	36.191	80.723	1.00 29.29
isi.		MOTA	3707	ND2	ASN A	466		39.775	37.015	82.111	1.00 28.19
4		ATOM	3708	N	ALA A	467		40.306	41.666	79.967	1.00 27.97
		MOTA	3709	CA	ALA A			40.587	43.079	80.295	1.00 26.66
10 ft.		ATOM	3710	С	ALA A			39.352	43.827	80.720	1.00 20.00
	30	MOTA	3711	0	ALA A			39.406	44.845	81.393	
n.		ATOM	3712	СВ	ALA A			41.365	43.837	79.256	1.00 31.71
12.00		ATOM	3713	N	CYS A			38.217	43.277		1.00 25.99
\$2 30°		ATOM	3714	CA	CYS A					80.336	1.00 28.06
14.64		ATOM	3715	C	CYS A			36.942	43.862	80.693	1.00 25.80
-4	35	ATOM	3716					36.668	43.619	82.165	1.00 26.47
	33	ATOM		O	CYS A			36.469	44.517	82.963	1.00 27.99
			3717	CB	CYS A			35.882	43.376	79.696	1.00 24.56
		ATOM	3718	SG	CYS A			36.455	43.873	78.049	1.00 27.76
		ATOM	3719	N	ILE A			36.752	42.384	82.540	1.00 24.34
	40	ATOM	3720	CA	ILE A			36.599	42.052	83.921	1.00 25.23
	40	ATOM	3721	C	ILE A			37.560	42.800	84.876	1.00 28.13
		ATOM	3722	0	ILE A			37.175	43.220	85.950	1.00 29.54
		ATOM	3723	CB	ILE A			36.858	40.574	84.068	1.00 27.23
		MOTA	3724		ILE A			35.956	39.801	83.112	1.00 26.94
	4.4	MOTA	3725	CG2	ILE A	469		36.537	40.208	85.496	1.00 25.56
	45	ATOM	3726	CD1	ILE A	469		36.247	38.298	83.085	1.00 45.50
		ATOM	3727	N	ALA A	470		38.830	42.960	84.534	1.00 23.28
		ATOM	3728	CA	ALA A	470		39.749	43.621	85.461	1.00 22.23
		ATOM	3729	С	ALA A			39.392	45.038	85.808	1.00 30.29
		MOTA	3730	0	ALA A			39.474	45.451	86.986	1.00 30.23
	50	MOTA	3731	CB	ALA A			41.218	43.502	85.074	1.00 32.82
		ATOM	3732	N	LEU A			39.007	45.760		
		ATOM	3733	CA	LEU A			38.643		84.759	1.00 23.53
		ATOM	3734	C	LEU A			37.333	47.173	84.834	1.00 18.39
		ATOM	3735	ō	LEU A				47.373	85.569	1.00 26.57
	55	ATOM	3736	CB	LEU A			37.210	48.208	86.462	1.00 30.48
	55	MOTA	3737					38.676	47.827	83.444	1.00 15.51
				CG	LEU A			38.671	49.325	83.539	1.00 24.20
		ATOM	3738		LEU A			39.754	49.795	84.513	1.00 24.86
		ATOM	3739		LEU A			38.876	49.941	82.156	1.00 26.35
	60	ATOM	3740	N	SER A			36.351	46.570	85.222	1.00 25.31
	60	ATOM	3741	CA	SER A			35.080	46.674	85.901	1.00 27.56
		ATOM	3742	С	SER A			35.260	46.477	87.396	1.00 33.46
		MOTA	3743	0	SER A	472		34.800	47.292	88.214	1.00 32.85
		ATOM	3744	CB	SER A	472		33.989	45.714	85.393	1.00 32.06
		MOTA	3745	OG	SER A	472		34.492	44.774	84.470	1.00 48.56
										= - =	

		ATOM	3746	N	GLN	А	473	35.911	45.350	87.736	1.00 27.52
		ATOM	3747	CA	GLN			36.170	44.971	89.108	1.00 24.10
		ATOM	3748	С	GLN			36.866	46.096	89.836	1.00 25.18
		ATOM	3749	0	GLN			36.534	46.458	90.969	1.00 21.62
	5	ATOM	3750	CB	GLN			36.994	43.671	89.148	1.00 25.86
	_	ATOM	3751	CG	GLN			36.128	42.402	89.118	1.00 32.72
		ATOM	3752	CD	GLN			34.970	42.504	90.090	1.00 46.08
		ATOM	3753		GLN			35.165	42.422	91.308	1.00 40.00
		ATOM	3754		GLN			33.761	42.692	89.559	1.00 40.73
	10	ATOM	3755	N	ARG			37.855	46.656	89.161	
	10	ATOM	3756	CA	ARG			38.562	47.765	89.779	1.00 24.00 1.00 24.46
	-	ATOM	3757	C	ARG			37.609			
			3758	0	ARG				48.893	90.141	1.00 29.31
		MOTA						37.620	49.447	91.242	1.00 33.13
	15	ATOM	3759	CB	ARG			39.682	48.290	88.898	1.00 20.19
	1.0	ATOM	3760	CG	ARG			40.866	47.352	88.831	1.00 28.48
		ATOM	3761	CD	ARG			41.871	47.869	87.832	1.00 34.41
		MOTA	3762	NE	ARG			42.258	49.245	88.093	1.00 40.09
		ATOM	3763	CZ	ARG			42.927	49.938	87.185	1.00 51.25
	20	MOTA	3764		ARG			43.220	49.376	86.019	1.00 24.79
13. 1	20	MOTA	3765		ARG			43.316	51.199	87.444	1.00 20.43
Halls.		MOTA	3766	N	TRP			36.791	49.259	89.178	1.00 25.32
		ATOM	3767	CA	TRP			35.862	50.332	89.400	1.00 26.77
135 MW		ATOM	3768	С	TRP			34.881	49.962	90.474	1.00 27.52
अंद्री सार्थ है असर		ATOM	3769	0	TRP		-	34.749	50.633	91.475	1.00 29.64
un -	25	MOTA	3770	CB	TRP			35.199	50.804	88.093	1.00 27.95
ļ.ā.		MOTA	3771	CG	TRP	Α	475	36.047	51.819	87.361	1.00 32.11
#		MOTA	3772	CD1	TRP	Α	475	36.873	51.592	86.298	1.00 35.65
<u>.</u>		MOTA	3773	CD2	TRP	Α	475	36.161	53.217	87.648	1.00 31.62
	×	MOTA	3774	NE1	TRP	Α	475	37.484	52.748	85.904	1.00 34.92
	30	MOTA	3775	CE2	TRP	Α	475	37.054	53.763	86.707	1.00 36.16
		ATOM	3776	CE3	TRP	Α	475	35.588	54.040	88.606	1.00 32.63
		ATOM	3777	CZ2	TRP	Α	475	37.372	55.112	86.719	1.00 36.24
		MOTA	37 7 8	CZ3	TRP	Α	475	35.897	55.375	88.616	1.00 34.74
in the		MOTA	3779	CH2	TRP	Α	475	36.777	55.901	87.685	1.00 35.77
3, 100	35	MOTA	3780	N	ILE	Α	476	34.234	48.847	90.279	1.00 26.36
		MOTA	3781	CA	ILE	Α	476	33.268	48.386	91.235	1.00 28.33
	-	MOTA	3782	С	ILE	Α	476	33.771	48.315	92.681	1.00 34.20
		MOTA	3783	0	ILE	A	476	33.056	48.595	93.637	1.00 36.89
		ATOM	3784	CB	ILE	Α	476	32.722	47.070	90.761	1.00 32.23
	40	ATOM	3785	CG1	ILE	Α	476	31.993	47.308	89.443	1.00 30.49
		MOTA	3786		ILE			31.864	46.376	91.851	1.00 34.86
		ATOM	3787	CD1	ILE	Α	476	31.595	46.005	88.756	1.00 33.04
		ATOM	3788	N	THR			35.010	47.934	92.860	1.00 27.27
		ATOM	3789	CA	THR			35.558	47.846	94.194	1.00 24.15
	45	ATOM	3790	С	THR			36.416	49.052	94.523	1.00 27.30
		ATOM	3791	0	THR			37.120	49.065	95.519	1.00 27.36
		ATOM	3792	СВ	THR			36.402	46.578	94.257	1.00 32.13
		ATOM	3793		THR			37.593	46.848	93.557	1.00 29.48
		ATOM	3794		THR			35.634	45.470	93.530	1.00 16.94
	50	ATOM	3795	N	ALA			36.371	50.097	93.695	1.00 22.33
		ATOM	3796	CA	ALA			37.164	51.260	93.988	1.00 20.44
		ATOM	3797	C	ALA			36.890	51.843	95.390	1.00 20.44
		ATOM	3798	ō	ALA			35.786	51.756	95.922	
		ATOM	3799	СВ	ALA			36.938	52.343	92.942	1.00 34.38 1.00 19.26
	55	ATOM	3800	N	LYS			37.931	52.469	95.970	
	, ,	ATOM	3801	CA	LYS			37.899			1.00 29.65
		ATOM	3802	C	LYS				53.168	97.243	1.00 27.30
		ATOM	3803					38.575	54.512	97.051	1.00 36.54
				O CB	LYS			39.378	54.692	96.118	1.00 34.13
	60	MOTA	3804	CB	LYS			38.457	52.410	98.417	1.00 28.01
	JU	ATOM	3805	CG	LYS			37.696	51.116	98.631	1.00 51.38
		ATOM	3806	CD	LYS			37.115		100.021	1.00 67.24
		ATOM	3807	-CE			479	35.804	50.103	99.931	1.00 87.12
		ATOM	3808	NZ			479	35.711		100.841	1.00 85.55
		ATOM	3809	N	GTO	A	480	38.241	55.477	97.900	1.00 36.30

		ATOM	3810	CA	GLU	Α	480	38.843	56.793	97.751	1.00 34.79
		ATOM	3811	С	GLU	Α	480	40.261	56.707	97.220	1.00 34.79
		MOTA	3812	0	GLU			40.613	57.332	96.234	1.00 34.10
		ATOM	3813	СВ	GLU			38.899	57.565	99.078	1.00 36.21
	5	ATOM	3814	CG	GLU			37.709	58.500	99.303	1.00 63.85
		ATOM	3815	CD	GLU			37.601	59.511	98.214	1.00100.00
		ATOM	3816	OE1	GLU			38.457	59.648	97.357	1.00100.00
		ATOM	3817		GLU			36.491	60.209	98.288	1.00100.00
		ATOM	3818	N	ASP			41.080	55.946	97.904	1.00 24.69
	10	ATOM	3819	CA	ASP			42.451	55.860	97.519	1.00 23.87
	10	ATOM	3820	C	ASP			42.771	55.314	96.132	1.00 23.87
			3821	Õ	ASP				55.312		
		ATOM						43.925		95.721	1.00 39.44
		ATOM	3822	CB	ASP			43.262	55.155	98.611	1.00 25.29
	15	MOTA	3823	CG	ASP			43.072	53.668	98.575	1.00 39.58
	15	MOTA	3824		ASP			42.471	53.029	97.708	1.00 46.00
		MOTA	3825		ASP			43.698	53.107	99.567	1.00 39.59
		MOTA	3826	N	ASP			41.788	54.881	95.373	1.00 30.70
		ATOM	3827	CA	ASP	Α	482	42.098	54.379	94.024	1.00 31.73
	1	ATOM	3828	С	ASP	Α	482	41.725	55.307	92.859	1.00 34.17
U.S.	20	ATOM	3829	0	ASP	A	482	42.158	55.150	91.717	1.00 35.45
The State of the S		ATOM	3830	CB	ASP	Α	482	41.399	53.022	93.756	1.00 33.31
5348 8 a -		MOTA	3831	CG	ASP	Α	482	41.686	51.970	94.779	1.00 38.90
-4. **		ATOM	3832	OD1	ASP	Α	482	42.810	51.514	94.992	1.00 42.45
15 21/2		ATOM	3833	OD2	ASP	Α	482	40.606	51.625	95.440	1.00 40.17
मर्चु मार इस्तर सर्वे मार	25	MOTA	3834	N	LEU	Α	483	40.863	56.246	93.146	1.00 29.93
a Figure	-	ATOM	3835	CA			483	40.352	57.159	92.160	1.00 27.80
2 770		ATOM	3836	C			483	41.434	57.943	91.410	1.00 40.70
		ATOM	3837	ŏ			483	41.386	58.102	90.180	1.00 40.76
181		ATOM	3838	СВ			483	39.265	58.049	92.819	1.00 22.54
	30	ATOM	3839	CG		-	483	38.148	57.240	93.488	1.00 20.75
	50	ATOM	3840		LEU			37.170	58.165	94.197	1.00 20.73
The state of		ATOM	3841		LEU			37.389	56.467	92.414	1.00 19.29
		MOTA	3842	N			484	42.410			
केम स्थाप स्थापन			3843	CA					58.446	92.162	1.00 36.15
is all	35	MOTA					484	43.459	59.225	91.571	1.00 34.08
###	33	ATOM	3844	C			484	44.168	58.524	90.429	1.00 39.51
		ATOM	3845	0			484	44.456	59.091	89.359	1.00 38.59
		ATOM	3846	CB			484	44.495	59.602	92.618	1.00 34.26
		ATOM	3847	CG			484	45.807	59.955	91.941	1.00100.00
	40	ATOM	3848		ASN			45.878	60.940	91.171	1.00100.00
	40	ATOM	3849		ASN			46.836	59.134	92.186	1.00100.00
		MOTA	3850	N			485	44.472	57.268	90.698	1.00 35.37
		ATOM	3851	CA			485	45.202	56.417	89.791	1.00 32.79
		ATOM	3852	С			485	44.522	56.140	88.484	1.00 32.26
	4-	MOTA	3853	0			485	45.159	55.925	87.463	1.00 32.44
	45	ATOM	3854	CB			485	45.565	55.132	90.477	1.00 38.65
		ATOM	3855	OG			485	46.040	55.437	91.777	1.00 62.66
		ATOM	3856	N			486	43.222	56.110	88.491	1.00 27.13
		ATOM	3857	CA	PHE	Α	486	42.631	55.809	87.233	1.00 28.26
		MOTA	3858	С			486	43.193	56.772	86.264	1.00 32.12
	50	ATOM	3859	0			486	43.423	57.910	86.604	1.00 32.02
		ATOM	3860	CB	PHE	Α	486	41.101	55.819	87.198	1.00 31.01
		MOTA	3861	CG	PHE	Α	486	40.471	54.807	88.132	1.00 27.04
		ATOM	3862	CD1	PHE	Α	486	40.504	53.425	87.911	1.00 22.43
		MOTA	3863	CD2	PHE	Α	486	39.805	55.293	89.253	1.00 21.40
	55	MOTA	3864		PHE			39.896	52.538	88.804	1.00 19.69
		ATOM	3865		PHE			39.224	54.426	90.174	1.00 19.20
		MOTA	3866	CZ			486	39.245	53.051	89.927	1.00 15.13
		ATOM	3867	N			487	43.455	56.279	85.089	1.00 34.97
		ATOM	3868	CA			487	44.032	57.092	84.070	1.00 34.06
	60	ATOM	3869	c			487	43.491	56.622	82.758	1.00 43.55
		ATOM	3870	Ö			487	42.951	55.537	82.604	1.00 45.33
		ATOM	3871	СВ			487	45.591	57.038	84.085	1.00 43.93
		MOTA	3872	CG			487	46.196	58.169	83.302	1.00 43.93
		ATOM	3873		ASN			46.057	58.189	82.077	1.00 36.10
		- 14 04 1				41	,	/	00.109	02.011	1.00 12.14

46.829 59.112 84.007 1.00 65.62

MOTA

3874 ND2 ASN A 487

	711011	2075		71011 11		40.029	33.112	04.007	1.00 05.02
	MOTA	3875	N	ALA A		43.662	57.435	81.781	1.00 39.34
	ATOM	3876	CA	ALA A		43.201	57.055	80.472	1.00 38.25
_	MOTA	3877	С	ALA A		44.024	55.900	79.809	1.00 43.58
5	MOTA	3878	0	ALA A	488	43.596	55.317	78.834	1.00 44.11
	ATOM	3879	СВ	ALA A		43.153	58.314	79.621	1.00 37.54
	ATOM	3880	N	THR A					
						45.207	55.555	80.314	1.00 38.34
	MOTA	3881	CA	THR A		45.996	54.499	79.715	1.00 36.16
	ATOM	3882	С	THR A	489	45.270	53.181	79.792	1.00 45.74
10	ATOM	3883	0	THR A	489	45.476	52.233	79.057	1.00 47.78
	ATOM	3884	CB	THR A		47.296	54.458	80.503	1.00 31.01
	ATOM	3885		THR A					
						46.961	54.457	81.872	1.00 35.33
	ATOM	3886	CG2	THR A		47.993	55.771	80.229	1.00 28.28
	ATOM	3887	N	ASP A	490	44.337	53.182	80.708	1.00 46.75
15	ATOM	3888	CA	ASP A		43.560	52.018	80.972	1.00 51.49
	ATOM	3889	C	ASP A		42.759			
							51.515	79.786	1.00 52.21
	ATOM	3890	0	ASP A		42.396	50.342	79.651	1.00 54.75
	ATOM	3891	CB	ASP A	490	42.676	52.345	82.184	1.00 54.04
	MOTA	3892	CG	ASP A	490	43.413	52.884	83.380	1.00 53.83
20	ATOM	3893	OD1	ASP A		44.621	52.777	83.616	1.00 62.93
	ATOM	3894		ASP A					
						42.565	53.446	84.165	1.00 35.66
	ATOM	3895	И	LEU A		42.486	52.450	78.938	1.00 42.42
	ATOM	3896	CA	LEU A	491	41.752	52.250	77.723	1.00 43.54
	ATOM	3897	С	LEU A	491	42.712	51.977	76.585	1.00 43.97
25	ATOM	3898	ō	LEU A					
20						42.340	51.438	75.588	1.00 42.53
	ATOM	3899	CB	LEU A		40.984	53.528	77.421	1.00 44.89
	ATOM	3900	CG	LEU A	491	39.794	53.747	78.338	1.00 48.31
	MOTA	3901	CD1	LEU A	491	38.558	54.171	77.552	1.00 49.16
	ATOM	3902		LEU A		39.377	52.494	79.125	
30		3903	N						1.00 39.24
30	MOTA			LYS A		43.958	52.403	76.754	1.00 42.32
	MOTA	3904	CA	LYS A		44.999	52.320	75.696	1.00 44.57
	ATOM	3905	С	LYS A	492	44.826	51.165	74.680	1.00 49.08
	ATOM	3906	0	LYS A	492	44.810	51.343	73.473	1.00 49.66
	ATOM	3907	CB	LYS A		46.359	52.177		
35	ATOM	3908						76.401	1.00 48.47
33			CG	LYS A		47.487	52.883	75.629	1.00 88.73
	ATOM	3909	CD	LYS A	492	48.852	52.537	76.197	1.00100.00
	ATOM	3910	CE	LYS A	492	48.786	51.460	77.300	1.00100.00
	ATOM	3911	NZ	LYS A	492	50.103	50.896	77.541	1.00100.00
	ATOM	3912	N	ASP A		44.711	49.917		
40								75.227	1.00 41.86
40	ATOM	3913	CA	ASP A		44.664	48.740	74.372	1.00 40.17
	ATOM	3914	С	ASP A		43.220	48.162	74.215	1.00 44.29
	MOTA	3915	0	ASP A	493	43.031	46.973	73.889	1.00 42.00
	ATOM	3916	CB	ASP A	493	45.560	47.699	75.015	1.00 41.52
	ATOM	3917	CG	ASP A		47.021			
45		3918					48.130	74.956	1.00 67.01
43	ATOM			ASP A		47.467	48.451	73.856	1.00 77.10
	MOTA	3919		ASP A		47.678	48.131	75.984	1.00 57.19
	ATOM	3920	N	LEU A	494	42.193	49.005	74.475	1.00 40.69
	ATOM	3921	CA	LEU A	494	40.789	48.512	74.526	1.00 36.32
	ATOM	3922	С	LEU A		39.992	48.877		
50	ATOM	3923	ō					73.245	1.00 37.76
50				LEU A		39.897	50.029	72.863	1.00 38.93
	ATOM	3924	CB	LEU A		40.098	49.125	75.733	1.00 32.52
	MOTA	3925	CG	LEU A	494	40.376	48.433	77.063	1.00 30.66
	ATOM	3926	CD1	LEU A	494	39.229	48.580	78.052	1.00 30.39
	ATOM	3927		LEU A					
55						40.611	46.925	76.918	1.00 23.54
33	ATOM	3928	N	SER A		39.477	47.825	72.631	1.00 25.56
	ATOM	3929	CA	SER A	495	38.674	48.017	71.457	1.00 22.23
	ATOM	3930	С	SER A	495	37.344	48.670	71.856	1.00 31.27
	ATOM	3931	0	SER A		36.968	48.706		
	ATOM	3932						73.038	1.00 31.21
60			CB	SER A		38.380	46.705	70.795	1.00 20.88
ou	ATOM	3933	OG	SER A	495	37.192	46.143	71.317	1.00 33.60
	ATOM	3934	N	SER A	496	36.627	49.184	70.865	1.00 29.48
	ATOM	3935	CA	SER A		35.363	49.821	71.139	
	ATOM	3936	C	SER A		34.495			1.00 26.67
							48.747	71.744	1.00 29.54
	ATOM	3937	0	SER A	490	33.744	48.960	72.697	1.00 24.80

	ATOM	3938	СВ	SER A	496	34.760	50.441	60 004	1 00	
	ATOM	3939	OG	SER A				69.894	1.00 2	
	ATOM	3940	N	HIS A		33.749	49.597	69.397	1.00	
						34.674	47.547	71.219	1.00 2	
5	ATOM	3941	CA	HIS A		33.949	46.383	71.750	1.00 2	
5	ATOM	3942	С	HIS A		34.156	46.148	73.275	1.00	37.24
	ATOM	3943	0	HIS A		33.238	45.863	74.041	1.00 3	
	ATOM	3944	CB	HIS A		34.364	45.106	70.978	1.00	
	ATOM	3945	CG	HIS A	497	34.182	45.348	69.545	1.00	
	ATOM	3946	ND1	HIS A	497	32.943	45.204	68.962	1.00	
10	ATOM	3947	CD2	HIS A	497	35.054	45.833	68.622	1.00	
	ATOM	3948	CE1	HIS A	497	33.075	45.531	67.702		
	ATOM	3949	NE2	HIS A	497	34.330	45.932	67.462	1.00 3	
	ATOM	3950	N	GLN A		35.406			1.00 3	
	ATOM	3951	CA	GLN A			46.243	73.715	1.00 3	
15	ATOM	3952	C			35.737	46.008	75.094	1.00 2	
1.0				GLN A		35.263	47.122	75.965	1.00 2	27.11
	ATOM	3953	0	GLN A		34.842	46.930	77.089	1.00 2	23.92
	ATOM	3954	CB	GLN A		37.221	45.659	75.248	1.00 2	29.95
	ATOM	3955	CG	GLN A		37.582	44.317	74.544	1.00 2	25.78
	MOTA	3956	CD	GLN A	498	39.074	44.084	74.535	1.00 2	
20	MOTA	3957	OE1	GLN A	498	39.796	44.891	73.960	1.00 2	
	MOTA	3958	NE2	GLN A	498	39.561	43.049	75.218	1.00 2	
	ATOM	3959	N	LEU A		35.289	48.301	75.431		
	ATOM	3960	CA	LEU A					1.00 2	
	ATOM	3961	C	LEU A		34.819	49.396	76.229	1.00 2	
25	ATOM	3962				33.351	49.162	76.632	1.00 2	
- 40			0	LEU A		32.893	49.361	77.780	1.00 2	29.41
	ATOM	3963	CB	LEU A		34.991	50.709	75.436	1.00 3	31.70
	ATOM	3964	CG	LEU A		36.242	51.512	75 .7 88	1.00 3	39.76
	ATOM	3965		LEU A		37.335	50.572	76.278	1.00 4	
20	ATOM	3966		LEU A	499	36.718	52.268	74.555	1.00 3	
30	ATOM	3967	N	ASN A	500	32.606	48.737	75.642	1.00 1	
	ATOM	3968	CA	ASN A	500	31.213	48.508	75.828	1.00 1	
	ATOM	3969	С	ASN A	500	30.919	47.455	76.864	1.00 1	
	MOTA	3970	0	ASN A		29.997	47.602	77.705	1.00 1	
	ATOM	3971	CB	ASN A		30.604	48.129	74.476		
35	ATOM	3972	CG	ASN A		29.093	48.214		1.00 1	
	ATOM	3973		ASN A		28.433		74.426	1.00 3	
	MOTA	3974	ND3	ASN A	500		49.151	74.930	1.00 3	
	ATOM	3975	N	GLU A		28.542	47.218	73.787	1.00 1	
	ATOM	3976	CA	GLU A		31.699	46.366	76.743	1.00 1	
40	ATOM	3977				31.626	45.224	77.625	1.00 1	
-10	ATOM		C	GLU A		31.948	45.676	79.063	1.00 2	
		3978	0	GLU A		31.175	45.463	80.009	1.00 2	5.02
	ATOM	3979	CB	GLU A		32.446	44.057	77.053	1.00 1	4.95
	MOTA	3980	CG	GLU A		32.371	42.827	77.989	1.00 3	
4.5	ATOM	3981	CD	GLU A	501	30.946	42.399	78.199	1.00 3	
45	ATOM	3982		GLU A		30.050	42.672	77.413	1.00 7	
	ATOM	3983	OE2	GLU A	501	30.780	41.694	79.292	1.00 4	
	ATOM	3984	N	PHE A	502	33.059	46.400	79.226	1.00 1	
	ATOM	3985	CA	PHE A		33.395	46.952	80.530	1.00 2	
	ATOM	3986	С	PHE A		32.179	47.679	81.125		
50	ATOM	3987	0	PHE A		31.786	47.491		1.00 2	
	ATOM	3988	СВ	PHE A		34.507		82.301	1.00 2	
	ATOM	3989	CG	PHE A			48.012	80.327	1.00 2	
	ATOM	3990				34.590	49.082	81.393	1.00 3	
				PHE A		35.085	48.781	82.662	1.00 2	
55	ATOM	3991		PHE A		34.211	50.402	81.132	1.00 3	9.16
33	ATOM	3992		PHE A		35.183	49.773	83.638	1.00 3	1.12
	ATOM	3993		PHE A		34.305	51.414	82.096	1.00 4	
	ATOM	3994	CZ	PHE A		34.812	51.090	83.352	1.00 3	
	ATOM	3995	N	LEU A	503	31.613	48.557	80.288	1.00 1	
	ATOM	3996	CA	LEU A		30.487	49.343	80.692	1.00 2	
60	ATOM	3997	С	LEU A		29.337	48.491	81.178	1.00 2	
	ATOM	3998	0	LEU A		28.768	48.784	82.243		
	ATOM	3999	СВ	LEU A		30.002	50.325	79.619	1.00 2	
	ATOM	4000	CG	LEU A		30.888			1.00 2	
	ATOM	4001		LEU A		30.000	51.571	79.465	1.00 2	1.47
	111 011	.001	~DI	TIPO M	JUJ	30.415	52.376	78.259	1.00 2	4.86

		MOTA	4002	CD2	LEU A	503	30.860	52.420	80.733	1.00 20.54
		ATOM	4003	N	ALA A	504	29.012	47.444	80.378	1.00 27.79
		ATOM	4004	CA	ALA A		27.911	46.474	80.643	
			4005	C						1.00 24.63
	E	ATOM			ALA A		28.140	45.752	81.939	1.00 27.71
	5	ATOM	4006	0	ALA A	504	27.265	45.577	82.817	1.00 28.62
		MOTA	4007	CB	ALA A	504	27.762	45.482	79.496	1.00 23.87
		ATOM	4008	N	GLN A	505	29.382	45.344	82.066	1.00 22.16
		ATOM	4009	CA	GLN A		29.738			
								44.710	83.299	1.00 21.02
	10	ATOM	4010	C	GLN A		29.489	45.737	84.423	1.00 31.26
	10	MOTA	4011	0	GLN A	505	28.787	45.507	85.413	1.00 32.31
		ATOM	4012	CB	GLN A	505	31.202	44.209	83.270	1.00 18.95
		ATOM	4013	CG	GLN A	505	31.367	42.881	82.495	1.00 13.72
		ATOM	4014	CD	GLN A		32.806			
								42.549	82.136	1.00 31.75
	1.5	ATOM	4015		GLN A		33.796	42.969	82.768	1.00 43.14
	15	ATOM	4016	NE2	GLN A	505	32.923	41.781	81.085	1.00 39.34
		ATOM	4017	N	THR A	506	30.056	46.918	84.263	1.00 25.95
		ATOM	4018	CA	THR A	506	29.855	47.864	85.302	1.00 23.64
:#F FB.		ATOM	4019	С	THR A		28.411			
								48.101	85.579	1.00 23.89
THE PARTY OF THE P	20	ATOM	4020	0	THR A		27.923	47.999	86.696	1.00 22.75
1.37	20	MOTA	4021	CB	THR A	506	30.600	49.130	85.008	1.00 23.72
र्वे स्था		MOTA	4022	OG1	THR A	506	31.938	48.749	84.742	1.00 27.18
He sty		ATOM	4023	CG2	THR A		30.502	49.961	86.260	1.00 11.12
102 207		ATOM	4024	N	LEU A		27.727	48.408	84.518	
200		ATOM	4025	CA	LEU A					1.00 17.92
	25		4026				26.334	48.683	84.604	1.00 17.22
#4 18	23	ATOM		С	LEU A		25.618	47.683	85.442	1.00 25.65
- A		ATOM	4027	0	LEU A		24.816	48.073	86.266	1.00 27.85
#		ATOM	4028	CB	LEU A	507	25.693	48.686	83.224	1.00 17.85
		ATOM	4029	CG	LEU A	507	24.207	48.930	83.336	1.00 21.02
1		ATOM	4030	CD1	LEU A	507	23.974	50.290	83.970	1.00 22.48
n,	30	ATOM	4031		LEU A		23.599	48.919	81.949	
		ATOM	4032	N	GLN A		25.878			1.00 15.25
\$20,00°								46.395	85.194	1.00 21.35
		ATOM	4033	CA	GLN A		25.215	45.333	85.979	1.00 18.08
E.		ATOM	4034	С	GLN A		25.386	45.561	87.508	1.00 34.24
ja it.	"	MOTA	4035	0	GLN A	508	24.653	45.017	88.343	1.00 34.04
14	35	ATOM	4036	CB	GLN A	508	25.713	43.917	85.608	1.00 10.94
		MOTA	4037	CG	GLN A		25.366	43.446	84.191	1.00 26.42
		ATOM	4038	CD	GLN A		25.635	41.944	84.002	1.00 52.93
		ATOM	4039	OE1	GLN A					
		ATOM	4040	NE2	GLN A		26.550	41.396	84.628	1.00 32.89
	40						24.864	41.252	83.147	1.00 34.36
	40	ATOM	4041	N	ARG A		26.380	46.361	87.901	1.00 33.73
		MOTA	4042	CA.	ARG A	509	26.600	46.614	89.328	1.00 32.53
		MOTA	4043	C	ARG A	509	26.153	48.016	89.727	1.00 33.63
		MOTA	4044	0	ARG A	509	26.509	48.522	90.777	1.00 31.08
		MOTA	4045	CB	ARG A		28.055	46.440	89.760	
	45	ATOM	4046	CG	ARG A					1.00 29.22
			4047				28.553	45.014	89.733	1.00 29.78
		ATOM		CD	ARG A		27.744	44.054	90.609	1.00 30.86
		ATOM	4048	NE	ARG A		28.533	43.602	91.756	1.00 82.23
		MOTA	4049	CZ	ARG A	509	29.842	43.274	91.726	1.00100.00
		ATOM	4050	NH1	ARG A	509	30.579	43.315	90.613	1.00 92.85
	50	ATOM	4051	NH2	ARG A	509	30.430	42.881	92.855	1.00 91.85
		MOTA	4052	N	ALA A		25.384	48.659	88.880	
		ATOM	4053	CA	ALA A					1.00 32.59
							24.952	49.985	89.215	1.00 32.51
		MOTA	4054	C	ALA A		24.151	49.845	90.479	1.00 34.97
		ATOM	4055	0	ALA A		23.601	48.785	90.693	1.00 37.57
	55	ATOM	4056	CB	ALA A	510	24.189	50.622	88.063	1.00 32.91
		ATOM	4057	N	PRO A	511	24.174	50.856	91.334	1.00 25.14
		MOTA	4058	CA	PRO A		24.867	52.102	91.052	1.00 21.00
		ATOM	4059	C	PRO A					
							26.217	52.178	91.694	1.00 29.23
	60	ATOM	4060	0	PRO A		26.445	51.601	92.723	1.00 28.16
	JU	ATOM	4061	CB	PRO A		24.102	53.169	91.818	1.00 21.55
		ATOM	4062	CG	PRO A	511	23.316	52.432	92.886	1.00 28.68
		ATOM	4063	CD	PRO A	511	23.169	50.995	92.407	1.00 25.16
		ATOM	4064	N	LEU A	512	27.094	52.968	91.109	1.00 32.95
		ATOM	4065	CA	LEU A		28.394	53.188	91.686	1.00 33.42
										UU JJ.4Z

	ATOM	4066	С	LEU A	512	28.	287	54.512	92.397	1.00	38.65
	ATOM	4067	0	LEU A	512	27.	388	55.305	92.114		40.69
	ATOM	4068	CB	LEU A	512		453	53.350	90.587		34.40
	ATOM	4069	CG	LEU A			178	52.049	90.216		40.13
5	ATOM	4070		LEU A			222	51.086	89.508		39.04
-	ATOM	4071		LEU A			322	52.385	89.273		
	ATOM	4072	N	PRO A							44.61
		4073					196	54.781	93.312		31.05
	ATOM		CA	PRO A			167	56.058	94.008		27.16
10	ATOM	4074	C	PRO A			296	57.203	93.019		23.76
10	ATOM	4075	0	PRO A			121	57.182	92.118	1.00	27.17
	ATOM	4076	CB	PRO A			387	56.013	94.948	1.00	25.59
	ATOM	4077	CG	PRO A	513	30.	702	54.542	95.149		27.14
	ATOM	4078	CD	PRO A	513	30.	030	53.779	94.032		25.00
	ATOM	4079	N	LEU A	514	28.	478	58.203	93.185		22.92
15	ATOM	4080	CA	LEU A	514		516	59.350	92.279		27.55
	ATOM	4081	С	LEU A			930	59.766	91.940		
	ATOM	4082	ŏ	LEU A			287				31.95
.89 pb.	ATOM	4083	СВ	LEU A				59.908	90.765		37.11
	ATOM	4084	CG				673	60.564	92.741		30.03
20				LEU A		27.		61.626	91.648		32.87
43 ZU	ATOM	4085	CD1			26.		61.082	90.440	1.00	28.48
La.	ATOM	4086		LEU A		26.		62.780	92.272	1.00	31.16
	ATOM	4087	N	GLY A	515	30.	731	59.989	92.979		24.42
HA HA	ATOM	4088	CA	GLY A	515	32.	131	60.384	92.811		25.59
1 A.	ATOM	4089	С	GLY A	515	32.		59.472	91.835		33.83
25	ATOM	4090	0	GLY A			746	59.914	91.035		35.67
jad.	ATOM	4091	N	HIS A		32.		58.180	91.891		
Pares.	MOTA	4092	CA	HIS A		33.					26.40
HI.	ATOM	4093	C	HIS A				57.255	90.998		25.86
in in	ATOM	4094				32.		57.578	89.560		27.62
□ 30			0	HIS A		33.		57.596	88.695	1.00	28.67
# # JU	ATOM	4095	CB	HIS A		32.		55.814	91.282	1.00	25.39
rj.	ATOM	4096	CG	HIS A		33.		55.283	92.505	1.00	27.96
124	ATOM	4097	NDl	HIS A	516	33.	6 35	56.092	93.602	1.00	30.14
17 F	ATOM	4098	CD2	HIS A	516	33.	929	54.037	92.791		27.79
	ATOM	4099		HIS A		34.	205	55.336	94.534		27.58
35	MOTA	4100	NE2	HIS A	516	34.	390	54.099	94.085		27.02
	ATOM	4101	N	ILE A		31.		57.815	89.315		21.40
	MOTA	4102	CA	ILE A		31.		58.107	87.973		22.75
	ATOM	4103	C	ILE A		31.		59.424	87.462		
	ATOM	4104	Õ	ILE A		32.		59.558	86.352		31.09
40	ATOM	4105	СB	ILE A							28.78
••	ATOM	4106		ILE A		29.		58.024	87.930		27.12
		4100				29.		56.610	88.312		29.40
	ATOM			ILE A		29.		58.285	86.536	1.00	25.49
	ATOM	4108		ILE A		29.		55.665	87.105	1.00	34.77
15	MOTA	4109	N	LYS A		31.		60.416	88.308	1.00	27.28
45	ATOM	4110	CA	LYS A		32.	108	61.690	87.955	1.00	23.77
* 4	ATOM	4111	С	LYS A		33.	558	61.482	87.485	1.00	24.03
	ATOM	4112	0	LYS A		33.	982	61.831	86.391		26.08
	ATOM	4113	CB	LYS A	518	32.	038	62.557	89.210		24.00
×	ATOM	4114	CG	LYS A	518	30.		63.060	89.591		19.24
50	ATOM	4115	CD	LYS A		30.		64.276	90.537		27.93
	ATOM	4116	CE	LYS A		29.		64.877	90.962		37.11
	ATOM	4117	NZ	LYS A		28.		65.988	90.104		
	ATOM	4118	N	ARG A							52.30
	ATOM	4119	CA	ARG A		34.		60.899	88.361		17.90
55	ATOM					35.		60.636	88.098		20.80
, 55		4120	C	ARG A		35.		59.874	86.802		28.98
	ATOM	4121	0	ARG A		36.		60.084	86.051		29.86
	ATOM	4122	СВ	ARG A		36.		59.844	89.276		20.56
	MOTA	4123	CG	ARG A		37.	721	59.308	89.036		29.02
	MOTA	4124	CD	ARG A	519	38.	668	60.320	88.404		41.17
60	ATOM	4125	NE	ARG A	519	40.		60.008	88.616		59.84
	ATOM	4126	CZ	ARG A		41.		60.858	88.349		50.77
	MOTA	4127		ARG A		40.		62.073	87.880		31.21
	ATOM	4128		ARG A		42.		60.486			
	ATOM	4129	N	MET A		34.			88.543		31.86
				31	J_ V	54.	, , ,	58.956	86.565	T.00	25.08

	ATOM	4130	CA	MET A	520	34.979	58.121	85.379	1.00 24.56
	MOTA	4131	С	MET A	520	34.906	58.918	84.086	1.00 29.37
	MOTA	4132	0	MET A	520	35.651	58.687	83.114	1.00 27.92
	MOTA	4133	CB	MET A	520	33.905	57.007	85.442	1.00 26.98
5	ATOM	4134	CG	MET A	520	34.082	55.902	84.399	1.00 28.02
	MOTA	4135	SD	MET A	520	32.830	54.591	84.479	1.00 27.87
	ATOM	4136	CE	MET A	520	33.246	53.825	86.070	1.00 22.09
	MOTA	4137	N	GLN A	521	33.982	59.864	84.067	1.00 28.32
	ATOM	4138	CA	GLN A	521	33.838	60.672	82.886	1.00 28.34
10	ATOM	4139	С	GLN A		35.067	61.540	82.785	1.00 36.52
	MOTA	4140	0	GLN A		35.514	61.879	81.707	1.00 35.87
	ATOM	4141	CB	GLN A	521	32.514	61.451	82.863	1.00 28.34
	MOTA	4142	CG	GLN A		32.564	62.774	82.079	1.00 9.68
	MOTA	4143	CD	GLN A		32.890	62.572	80.616	1.00 27.55
15	ATOM	4144		GLN A		33.382	63,491	79.924	1.00 28.25
10	ATOM	4145		GLN A		32.657	61.368	80.142	1.00 25.70
	ATOM	4146	N	GLU A		35.626	61.827	83.963	1.00 25.70
	ATOM	4147	CA	GLU A		36.818	62.648	84.171	1.00 36.13
	ATOM	4148	c.	GLU A		38.136	62.046	83.662	1.00 30.13
20	ATOM	4149	Ö	GLU A		39.099	62.735	83.335	
20	ATOM	4150	СВ	GLU A		36.857	63.035	85.641	1.00 42.40
		4151	CG	GLU A					1.00 37.79
	MOTA					38.233	63.196	86.273	1.00 58.85
	ATOM	4152	CD	GLU A		38.046	64.040	87.493	1.00 73.64
25	ATOM	4153		GLU A		37.006	64.641	87.709	1.00 45.66
25	MOTA	4154		GLU A		39.081	64.037	88.289	1.00 47.91
	ATOM	4155	N	VAL A		38.188	60.739	83.552	1.00 40.13
	ATOM	4156	CA	VAL A		39.401	60.136	83.058	1.00 37.49
	ATOM	4157	С	VAL A		39.205	59.351	81.778	1.00 38.88
20	ATOM	4158	0	VAL A		40.195	59.016	81.138	1.00 40.21
30	ATOM	4159	CB	VAL A		40.184	59.370	84.102	1.00 40.01
	ATOM	4160		VAL A		40.231	60.165	85.413	1.00 39.12
	MOTA	4161		VAL A		39.534	58.017	84.320	1.00 39.82
	MOTA	4162	N	TYR A		37.952	59.048	81.379	1.00 30.35
~ -	ATOM	4163	CA	TYR A		37.801	58.330	80.114	1.00 28.11
35	MOTA	4164	С	TYR A		37.061	59.144	79.074	1.00 33.14
	MOTA	4165	0	TYR A		37.076	58.802	77.908	1.00 35.84
	ATOM	4166	CB	TYR A	524	37.281	56.878	80.119	1.00 25.56
	ATOM	4167	CG	TYR A		37.941	55.960	81.111	1.00 20.87
	ATOM	4168		TYR A		39.324	55.938	81.258	1.00 21.59
40	ATOM	4169		TYR A		37.170	55.083	81.879	1.00 19.80
	MOTA	4170	CE1	TYR A	524	39.905	55.063	82.176	1.00 25.64
	MOTA	4171	CE2	TYR A		37.731	54.227	82.827	1.00 18.61
	ATOM	4172	CZ	TYR A	524	39.116	54.231	82.969	1.00 19.81
	MOTA	4173	OH	TYR A		39.706	53.402	83.863	1.00 23.92
45	ATOM	4174	N	ASN A	525	36.416	60.221	79.496	1.00 25.98
	ATOM	4175	CA	ASN A	525	35.687	61.088	78.588	1.00 25.01
	MOTA	4176	С	ASN A	525	34.661	60.354	77.735	1.00 29.86
	ATOM	4177	0	ASN A	525	34.533	60.535	76.499	1.00 29.39
	MOTA	4178	CB	ASN A	525	36.637	61.922	77.739	1.00 29.55
50	MOTA	4179	CG	ASN A	525	35.949	62.980	76.894	1.00 30.32
	ATOM	4180	OD1	ASN A	525	36.460	63.332	75.850	1.00 32.77
	MOTA	4181	ND2	ASN A	525	34.822	63.527	77.344	1.00 13.80
	ATOM	4182	N	PHE A	526	33,924	59.512	78.436	1.00 24.21
	ATOM	4183	CA	PHE A	526	32.900	58.745	77.807	1.00 25.14
55	MOTA	4184	С	PHE A	526	31.846	59.631	77.214	1.00 31.74
	ATOM	4185	0	PHE A		31.161	59.241	76.272	1.00 34.99
	ATOM	4186	CB	PHE A		32.256	57.732	78.781	1.00 26.60
	ATOM	4187	CG	PHE A		33.115	56.499	78.978	1.00 23.82
	ATOM	4188		PHE A		34.017	56.080	78.000	1.00 25.00
60	MOTA	4189		PHE A		33.031	55.767	80.159	1.00 23.00
	ATOM	4190		PHE A		34.783	54.927	78.173	1.00 27.63
	ATOM	4191		PHE A		33.817	54.634	80.370	1.00 27.03
	MOTA	4192	CZ	PHE A		34.683	54.202	79.364	1.00 25.28
	ATOM	4193	N	ASN A		31.689	60.815	77.760	1.00 28.22
	,			1			55.015		2.00 20.22

To see that the see that the see that the see that the see the see the see the see that the see the se

		14			_						
		MOTA	4194	CA	ASN A	527	30.657	61.688	77.214	1.00	31.18
		ATOM	4195	С	ASN A	527	30.884	62.046	75.744	1.00	33.17
		ATOM	4196	0	ASN A	527	29.965	62.394	74.999	1.00	30.80
		MOTA	4197	CB	ASN A		30.479	62.967	78.052		36.41
	5	ATOM	4198	CG	ASN A		29.638	62.752			46.99
	,								79.292		
		MOTA	4199		ASN A		29.647	63.571	80.209		36.82
		ATOM	4200	ND2	ASN A	527 .	28.922	61.636	79.338		43.55
		MOTA	4201	N	ALA A	528	32.136	61.947	75.348	1.00	27.46
		MOTA	4202	CA	ALA A	528	32.581	62.278	74.005		26.48
	10	MOTA	4203	С	ALA A		32.335	61.188	72.950		32.09
	10										
		MOTA	4204	0	ALA A		32.420	61.404	71.753		32.09
		MOTA	4205	CB	ALA A		34.076	62.584	74.105	1.00	26.04
		MOTA	4206	N	ILE A	529	32.067	59.983	73.402	1.00	31.35
		ATOM	4207	CA	ILE A	529	31.854	58.859	72.529	1.00	28.47
	15	MOTA	4208	С	ILE A	529	30.492	58.904	71.887		35.96
	× 1	ATOM	4209	0	ILE A		29.486	59.023	72.578		38.79
		ATOM	4210	CB	ILE A		32.103	57.544	73.264		30.17
		ATOM	4211		ILE A		33.622	57.291	73.392		31.37
74 FE		ATOM	4212	CG2	ILE A	529	31.428	56.411	72.489	1.00	27.63
de to	20	ATOM	4213	CD1	ILE A	529	34.059	56.515	74.635		33.41
		ATOM	4214	N	ASN A		30.462	58.806	70.559		34.86
100			4215		ASN A						
J.E.		ATOM		CA			29.196	58.841	69.852		36.44
1200		- ATOM	4216	С	asn a		28.596	57.495	69.473		39.90
	7	ATOM	4217	0	ASN A	530	27.452	57.437	69.043	1.00	41.37
हम्मः सर्वेकाः	25	ATOM	4218	CB	ASN A	530	28.951	60.044	68.928		51.44
		ATOM	4219	CG	ASN A	530	28.461	61.253	69.732		100.00
44. 14.		ATOM	4220		ASN A		27.652				
]=£.								61.109	70.665		100.00
#		MOTA	4221		ASN A		28.955	62.442	69.392		91.39
	•	MOTA	4222	N	ASN A		29.368	56.403	69.688	1.00	30.37
H. 113	30	MOTA	4223	CA	ASN A	531	28.912	55.030	69.446	1.00	28.14
T.		MOTA	4224	С	ASN A	531	27.696	54.753	70.360	1.00	32.80
n.		MOTA	4225	0	ASN A		27.746	54.887	71.611		36.74
\$2.20°		ATOM	4226	СВ	ASN A						
12.20							30,092	54.066	69.690		24.31
	25	ATOM	4227	CG	ASN A		29.770	52.601	69.730		34.44
1.4.	35	ATOM	4228	OD1	ASN A	531	28.795	52.182	70.359	1.00	36.49
4-200		MOTA	4229	ND2	ASN A	531	30.643	51.810	69.099	1.00	30.57
		ATOM	4230	N	SER A	532	26.570	54.403	69.734		22.02
		ATOM	4231	CA	SER A		25.325	54.183	70.459		19.67
		ATOM	4232	c	SER A		25.323				
	40							53.208	71.627		26.15
	40	ATOM	4233	0	SER A		24.767	53.475	72.680		26.64
		MOTA	4234	CB	SER A	532	24.090	54.034	69.582	1.00	26.92
		ATOM	4235	OG	SER A	532	24.294	53.211	68.452	1.00	23.59
		MOTA	4236	N	GLU A	533	25.929	52.062	71.423		22.68
		ATOM	4237	CA	GLU A	533	25.995	51.036	72.420		22.97
	45	ATOM	4238	C	GLU A		26.677	51.569	73.635		
											30.48
		MOTA	4239	0	GLU A		26.125	51.539	74.749		31.13
		MOTA	4240	СВ	GLU A		26.683	49.779	71.850		23.96
		MOTA	4241	CG	GLU A	533	25.827	49.146	70.733	1.00	20.82
		MOTA	4242	CD	GLU A	533	24.611	48.450	71.276		40.65
	50	MOTA	4243	OE1	GLU A	533	24.432	48.256	72.476		36.25
	_	ATOM	4244		GLU A		23.782			1 00	25.23
								48.038	70.339		25.87
		ATOM	4245	N	ILE A		27.872	52.101	73.392		26.20
		MOTA	4246	CA	ILE A		28.622	52.672	74.484		26.32
		ATOM	4247	C	ILE A	534	27.900	53.849	75.121	1.00	27.83
	55-	ATOM	4248	0	ILE A	534	27.697	53.911	76.326		26.54
		ATOM	4249	CB	ILE A		30.051	53.022	74.102		29.16
		ATOM	4250		ILE A					1 00	20.10
							30.738	51.808	73.479	1.00	29.47
		MOTA	4251		ILE A		30.801	53.458	75.353		28.28
		MOTA	4252	CD1	ILE A		32.038	52.184	72.765	1.00	34.99
	60	ATOM	4253	N	ARG A	535	27.480	54.805	74.320		24.30
		ATOM	4254	CA	ARG A		26.804	55.898	74.949	1.00	22.51
		ATOM	4255	C	ARG A		25.573	55.401	75.701		28.19
		MOTA	4256	Ö	ARG A						
							25.212	55.808	76.791		32.61
		MOTA	4257	CB	ARG A	232	26.457	56.942	73.913	1.00	24.83

	ATOM	4258	CG	ARG I	4 535		25.970	58.229	74 547	1 00	01 40
	ATOM	4259	CD	ARG A			25.370		74.541		21.49
	ATOM	4260	NE	ARG A			25.194	59.183 60.457	73.554		13.79
	ATOM	4261	CZ	ARG I			26.256		74.213		31.38
5	ATOM	4262		ARG A			27.463	61.140 60.677	74.554		29.41
	ATOM	4263		ARG A					74.259		26.45
	ATOM	4264	N		4 536		26.110	62.302	75.195		19.99
	ATOM	4265	CA	PHE A		•	24.911	54.466	75.126		23.44
	ATOM	4266					23.740	53.980	75.770		22.05
10			C	PHE A			23.976	53.555	77.199		22.74
10	ATOM	4267	0	PHE A			23.349	54.113	78.105		22.06
	ATOM	4268	CB	PHE A			23.117	52.865	74.919	1.00	23.17
	ATOM	4269	CG	PHE A			22.040	52.153	75.658	1.00	21.92
	ATOM	4270		PHE A			20.933	52.845	76.150	1.00	22.66
1.5	ATOM	4271		PHE A			22.145	50.783	75.882	1.00	23.25
15	ATOM	4272	CE1	PHE A			19.926	52.181	76.847		21.23
	ATOM	4273	CE2				21.147	50.101	76.576		24.70
	ATOM	4274	CZ	PHE A	A 536		20.047	50.811	77.065		20.57
	ATOM	4275	N	ARG A	¥ 537		24.863	52.560	77.364		18.22
	ATOM	4276	CA	ARG A	537		25.239	51.995	78.665		19.20
20	ATOM	4277	С	ARG A	537		25.932	52.963	79.618		27.62
	ATOM	4278	0	ARG A			25.803	52.845	80.837		
	ATOM	4279	СВ	ARG A			26.035	50.709	78.556		26.73
	ATOM	4280	CG	ARG A			25.318	49.656	77.708		18.91
	ATOM	4281	CD	ARG A			26.181				16.55
25	ATOM	4282	NE	ARG A			25.341	48.426	77.387		21.58
	ATOM	4283	CZ	ARG A				47.357	76.886		28.42
	ATOM	4284	NH1				25.060	47.206	75.609		18.29
	ATOM	4285					25.569	48.004	74.703		22.46
				ARG A			24.240	46.236	75.224		25.22
30	ATOM	4286	N	TRP A			26.668	53.930	79.064		24.21
30	ATOM	4287	CA	TRP F			27.337	54.918	79.867	1.00	22.11
	ATOM	4288	C	TRP A			26.274	55.719	80.550	1.00	28.09
	ATOM	4289	0	TRP A			26.320	55.951	81.741		27.39
	ATOM	4290	CB	TRP A			28.064	55.888	78.949		20.48
35	ATOM	4291	CG	TRP A			28.606	57.157	79.580	1.00	21.29
33	ATOM	4292		TRP A			28.641	58.345	78.968		22.86
	ATOM ATOM	4293 4294	CD2				29.286	57.352	80.845	1.00	21.79
	ATOM	4295	NE1 CE2	-			29.228	59.270	79.769	1.00	22.70
	ATOM	4296	CE3				29.643	58.696	80.911		24.79
40	ATOM	4297					29.574	56.535	81.946		23.35
-10	ATOM		CZ2	_			30.280	59.248	82.025		25.89
		4298	CZ3				30.203	57.056	83.046		23.35
	ATOM	4299	CH2				30.562	58.405	83.081	1.00	24.89
	ATOM	4300	N	LEU A			25.303	56.161	79.758		27.31
45	ATOM	4301	CA	LEU A			24.229	56.974	80.306	1.00	27.18
42	MOTA	4302	C	LEU A			23.369	56.245	81.332		28.25
	ATOM	4303	0	LEU A			22.857	56.822	82.266	1.00	27.19
	ATOM	4304	CB	LEU A			23.428	57.812	79.262	1.00	26.37
	ATOM	4305	CG	LEU A	539		24.269	58.682	78.279	1.00	25.71
50	ATOM	4306		LEU A			23.369	59.424	77.290	1.00	21.79
30 ,	ATOM	4307		LEU A			25.146	59.680	79.011	1.00	23.51
	ATOM	4308	N	ARG A			23.199	54.960	81.188		27.56
	ATOM	4309	CA	ARG A			22.390	54.283	82.170	1.00	26.88
	ATOM	4310	С	ARG A			23.145	54.229	83.453		31.82
55	ATOM	4311	0	ARG A			22.618	54.448	84.539		32.72
55	MOTA	4312	CB	ARG A	540		22.034	52.888	81.732		24.48
	ATOM	4313	CG	ARG A			21.447	52.885	80.331	1.00	32.96
	ATOM	4314	CD	ARG A	540		20.695	51.597	80.090		33.19
	MOTA	4315	NE	ARG A			19.660	51.414	81.085		33.19
-	ATOM	4316	CZ	ARG A	540		19.151	50.242	81.409		30.83
60	MOTA	4317	NH1	ARG A			19.564	49.132	80.849		25.37
	MOTA	4318		ARG A			18.186	50.186	82.317		
	ATOM	4319	N	LEU A			24.414	53.948	83.318		30.30
	ATOM	4320	CA	LEU A			25.239	53.895	84.505		28.93
	ATOM	4321	C	LEU A			25.036	55.210	85.277	1.00	26.36
			1					33.210	03.211	1.00	31.00

		T COM	4222	^	TEH N	E 4 1	24 622	EE 046	06 430	1 00 21 62
		ATOM	4322	0	LEU A		24.632	55.246	86.439	1.00 31.62
		ATOM	4323	СВ	LEU A		26.702	53.586	84.094	1.00 23.61
		MOTA	4324	CG	LEU A		27.730	53.533	85.212	1.00 24.67
		ATOM	4325	CD1	LEU A	541	27.387	52.411	86.190	1.00 25.02
	5	ATOM	4326	CD2	LEU A	541	29.098	53.245	84.621	1.00 19.31
		ATOM	4327	N	CYS A	542	25.254	56.307	84.570	1.00 30.52
		ATOM	4328	CA	CYS A	542	25.115	57.661	85.105	1.00 31.76
		ATOM	4329	С	CYS A		23.808	57.996	85.805	1.00 32.71
		ATOM	4330	ō	CYS A		23.801	58.536	86.914	1.00 33.97
	10	ATOM	4331	СВ	CYS A		25.461	58.744	84.073	
	10									1.00 31.30
		MOTA	4332	SG	CYS A		27.085	58.488	83.347	1.00 34.39
		ATOM	4333	N	ILE A		22.711	57.708	85.125	1.00 25.61
		MOTA	4334	CA	ILE A		21.382	57.982	85.643	1.00 23.12
		MOTA	4335	С	ILE A	543	21.199	57.161	86.885	1.00 30.15
	15	MOTA	4336	0	ILE A	543	20.900	57.645	87.972	1.00 30.73
		ATOM	4337	CB	ILE A	543	20.340	57.627	84.585	1.00 23.75
		ATOM	4338	CG1	ILE A		20.369	58.664	83.468	1.00 24.09
		ATOM	4339		ILE A		18.955	57.572	85.182	1.00 22.99
Ser.		MOTA	4340		ILE A		20.386	60.109	83.982	1.00 27.34
	20		4341		GLN A					
dia.	20	ATOM		N			21.440	55.884	86.695	1.00 27.99
To est		ATOM	4342	CA	GLN A		21.320	54.929	87.756	1.00 25.72
-		MOTA	4343	С	GLN A		22.243	55.269	88.901	1.00 26.34
E 4794.		MOTA	4344	0	GLN A	. 544	22.029	54.826	90.014	1.00 26.24
THE THE		MOTA	4345	CB	GLN A	544	21.562	53.512	87.210	1.00 26.76
12 FF4.	25	ATOM	4346	CG	GLN A	. 544	20.355	52.955	86.432	1.00 17.74
144		ATOM	4347	CD	GLN A	544	20.598	51.604	85.743	1.00 32.62
- E		MOTA	4348	OE1	GLN A		20.326	51.432	84.551	1.00 38.66
3		ATOM	4349		GLN A		21.063	50.627	86.494	1.00 14.93
#			4350		SER A			56.033		
- A.	30	ATOM		N			23.286		88.625	1.00 21.73
	20	MOTA	4351	CA	SER A		24.187	56.392	89.685	1.00 22.42
FF R		ATOM	4352	С	SER A		23.819	57.726	90.287	1.00 33.67
		ATOM	4353	0	SER A		24.567	58.257	91.133	1.00 37.22
		MOTA	4354	CB	SER A	545	25.646	56.322	89.338	1.00 21.57
12.00	- 1	ATOM	4355	OG	SER A	545	25.980	[^] 54.968	89.163	1.00 31.72
las die	35	ATOM	4356	N	LYS A	546	22.662	58.251	89.841	1.00 23.09
Harana And		MOTA	4357	CA	LYS A	. 546	22.135	59.490	90.356	1.00 20.79
		ATOM	4358	C	LYS A		22.887	60.738	89.961	1.00 27.55
		ATOM	4359	0	LYS A		23.001	61.655	90.771	1.00 27.95
		ATOM	4360	СВ	LYS A		22.126	59.449	91.881	1.00 27.33
	40	ATOM	4361	CG	LYS A					
	1 0						21.498	58.195	92.484	1.00 15.90
		MOTA	4362	CD	LYS A		20.245	57.814	91.731	1.00 39.84
		ATOM	4363	CE	LYS A		19.355	56.850	92.498	1.00 45.16
		ATOM	4364	NZ	LYS A		18.197	56.399	91.704	1.00 40.14
		MOTA	4365	N	TRP A	547	23.414	60.776	88.753	1.00 23.26
	45	ATOM	4366	CA	TRP A	547	24.141	61.931	88.289	1.00 21.90
		MOTA	4367	С	TRP A	547	23.221	62.901	87.570	1.00 29.82
		ATOM	4368	0	TRP A	547	22.808	62.679	86.432	1.00 34.91
		ATOM	4369	СВ	TRP A		25.262	61.500	87.361	1.00 21.04
		MOTA	4370	CG	TRP A		26.254	62.591	87.206	1.00 22.57
	50	ATOM	4371		TRP A		26.224	63.769	87.844	1.00 25.87
		ATOM	4372		TRP A		27.437	62.588	86.417	
			4373		TRP A					1.00 23.40
		ATOM					27.316	64.511	87.517	1.00 25.64
		ATOM	4374		TRP A		28.081	63.819	86.635	1.00 27.46
		MOTA	4375		TRP P		28.014	61.668	85.547	1.00 26.21
	55	ATOM	4376		TRP A		29.279	64.162	85.995	1.00 27.44
		ATOM	4377		TRP A		29.195	62.009	84.923	1.00 28.70
		MOTA	4378	CH2	TRP P	547	29.822	63.236	85.138	1.00 28.41
		MOTA	4379	N	GLU A		22.888	63.995	88.227	1.00 22.95
		ATOM	4380	CA	GLU P		21.979	64.970	87.649	1.00 20.70
	60	ATOM	4381	C	GLU P		22.419	65.473	86.305	1.00 28.32
	.55	ATOM	4382	õ	GLU F					
							21.598	65.735	85.391	1.00 29.41
		ATOM	4383	CB	GLU A		21.635	66.144	88.607	1.00 22.45
		ATOM	4384	CG	GLU A		20.884	65.709	89.919	1.00 30.56
		ATOM	4385	CD	GLU A	1 548	20.337	66.848	90.765	1.00 59.35

	ATOM	4386		GLU A		20.336	68.021	90.413	1.00 8	
	ATOM	4387		GLU A		19.888	66.450	91.925	1.00 5	
	ATOM	4388	N	ASP A		23.728	65.661	86.201	1.00 2	
0	ATOM	4389	CA	ASP A		24.276	66.190	84.981	1.00 2	
5	ATOM	4390	C	ASP A		23.914	65.359	83.795	1.00 3	
	MOTA	4391	0	ASP A		23.760	65.869	82.697	1.00 3	
	ATOM	4392	CB	ASP A		25.775	66.480	85.048	1.00 2	
	ATOM	4393	CG	ASP A		26.076	67.463	86.130	1.00 3	
10	ATOM	4394		ASP A		25.432	68.479	86.297	1.00 4	
10	ATOM	4395		ASP A		27.076	67.115	86.882	1.00 4	
	ATOM	4396	N	ALA A		23.766	64.073	84.032	1.00 2	
	ATOM	4397	CA	ALA A		23.445	63.133	82.965	1.00 2	
	ATOM	4398	C	ALA A		22.019	63.171	82.431	1.00 3	
15	MOTA	4399	O	ALA A		21.745	62.615	81.361	1.00 3	
13	ATOM	4400	CB	ALA A		23.812	61.713	83.372	1.00 2	
	ATOM	4401	N	ILE A		21.123	63.795	83.192	1.00 2	
	ATOM	4402	CA	ILE A		19.716	63.882	82.832	1.00 2	
	ATOM	4403 4404	С 0	ILE A		19.461	64.355	81.411	1.00 3	
20	ATOM ATOM	4405	CB	ILE A		18.833 18.876	63.679	80.619	1.00 3	
20	ATOM	4406	CG1			19.038	64.641	83.868 85.226	1.00 3	
	ATOM	4407	CG2	ILE A		17.391	63.985 64.661		1.00 3	
	ATOM	4408		ILE A		18.072		83.475 86.253	1.00 2	
	ATOM	4409	N	PRO A		19.969	64.561 65.529		1.00 3	
25	ATOM	4410	CA	PRO A		19.793	66.121	81.099	1.00 3	
	ATOM	4411	C	PRO F		20.240	65.224	79.796 78.669	1.00 3	
	ATOM	4412	ō	PRO A		19.583	65.119	77.622	1.00 3	
	ATOM	4413	СВ	PRO F		20.659	67.383	79.787	1.00 2	
	MOTA	4414	CG	PRO P		21.348	67.500	81.139	1.00 3	
30	ATOM	4415	CD	PRO A		20.934	66.296	81.950	1.00 3	
	ATOM	4416	N	LEU A		21.391	64.616	78.891	1.00 2	
	ATOM	4417	CA	LEU A		21.997	63.727	77.931	1.00 2	
y ===	ATOM	4418	C	LEU A		21.138	62.522	77.670	1.00 3	
	ATOM	4419	0	LEU A		21.015	62.087	76.523	1.00 3	
35	ATOM	4420	СВ	LEU A		23.362	63.281	78.439	1.00 2	
	ATOM	4421	CG	LEU A		24.196	64.496	78.818	1.00 2	
	ATOM	4422	CD1			25.608	64.071	79.174	1.00 1	
	MOTA	4423	CD2	LEU A		24.188	65.479	77.630	1.00 1	
1	ATOM	4424	N	ALA A	554	20.563	61.973	78.754	1.00 3	
40	MOTA	4425	CA	ALA A	554	19.726	60.779	78.669	1.00 2	
	ATOM	4426	С	ALA A	554	18.432	61.107	77.988	1.00 3	
	MOTA	4427	0	ALA A	554	17.944	60.332	77.163	1.00 3	37.08
	ATOM	4428	CB	ALA A		19.475	60.165	80.017	1.00 2	26.78
4.5	ATOM	4429	N	LEU A		17.898	62.283	78.320	1.00 2	29.70
45	ATOM	4430	CA	LEU A		16.644	62.724	77.720	1.00 2	28.32
	MOTA	4431	С	LEU A		16.803	62.902	76.229	1.00 2	29.19
	ATOM	4432	0	LEU A		15.970	62.506	75.385	1.00 2	26.13
	ATOM	4433	CB	LEU A		16.110	64.027	78.342	1.00 2	
50	ATOM	4434	CG	LEU A		15.371	63.814	79.666	1.00 3	
50	MOTA	4435		LEU A		15.360	65.118	80.464	1.00 3	
	ATOM	4436		LEU A		13.938	63.334	79.427	1.00 2	
	ATOM	4437	N	LYS A		17.922	63.524	75.950	1.00 2	
	ATOM	4438	CA	LYS A		18.325	63.839	74.615	1.00 2	
55	MOTA	4439	С	LYS A		18.369	62.591	73.800	1.00 3	
ا رر	ATOM	4440	O	LYS A		17.670	62.491	72.796	1.00 4	
	ATOM	4441	CB	LYS A		19.645	64.592	74.599	1.00 3	
	ATOM	4442	CG	LYS A		20.101	65.139	73.250	1.00	
	ATOM	4443	CD	LYS A		21.585	65.518	73.254	1.00 8	
60	ATOM	4444	CE NZ	LYS A		22.046	66.270	72.011	1.00	
50	ATOM	4445	NZ	LYS A		23.239	65.661	71.401	1.00	
	ATOM	4446	N	MET A		19.154	61.623	74.248	1.00 2	
	ATOM	4447	CA C	MET A		19.305	60.364	73.514	1.00 2	
	ATOM	4448	0	MET A		18.033	59.553	73.287	1.00	
	ATOM	4449	J	ribi F	3 331	17.811	58.907	72.263	1.00 2	23.24

		ATOM	4450	CB	MET A	A 55	7	20.401	59.488	74.104	1.00 24.89
		ATOM	4451		MET A			20.533		73.368	1.00 29.37
		ATOM	4452	SD	MET A	A 55	7	22.029	57.276	73.864	1.00 33.21
		ATOM	4453	CE	MET A	A 55	7	21.939	55.812	72.793	1.00 30.16
	5	ATOM	4454	N	ALA A	A 55	8	17.203	59.568	74.287	1.00 33.42
		ATOM	4455	CA	ALA A	A 55	8	16.000	58.816	74.194	1.00 33.03
		ATOM	4456	С	ALA A	A 55	8	15.042	59.345	73.163	1.00 38.12
		ATOM	4457	0	ALA A	A 55	8	14.349	58.568	72.543	1.00 37.09
		MOTA	4458	CB	ALA A	A 55	8	15.317	58.780	75.553	1.00 32.89
	10	ATOM	4459	N	THR A	A 55	9	14.994	60.665	73.032	1.00 36.76
		ATOM	4460	CA	THR A	A 55	9	14.067	61.326	72.144	1.00 36.43
		ATOM	4461	С	THR A	A 55	9	14.588	61.590	70.794	1.00 41.71
		MOTA	4462	0	THR A	A 55	9	13.788	61.768	69.891	1.00 44.66
		MOTA	4463	CB	THR A	A 55	59	13.615	62.705	72.694	1.00 43.70
	15	MOTA	4464	OG1	THR A	A 55	59	14.728	63.545	72.957	1.00 38.88
		ATOM	4465	CG2	THR A			12.764	62.549	73.942	1.00 44.95
		MOTA	4466	N	GLU 1	A 56	50	15.897	61.695	70.674	1.00 37.38
1 15-		ATOM	4467	CA	GLU A	A 56	50	16.495	62.018	69.395	1.00 36.51
34.00		ATOM	4468	C	GLU 1	A 56	50	16.652	60.846	68.448	1.00 40.11
10 m	20	MOTA	4469	0	GLU 1	A 56	50	17.003	61.052	67.300	1.00 43.23
		ATOM	4470	CB	GLU 1	A 56	50	17.799	62.820	69.519	1.00 38.13
\$=£:		ATOM	4471	CG	GLU J	A 56	50	17.653	64.142	70.292	1.00 54.29
124		ATOM	4472	CD	GLU I	A 56	50	18.857	65.043	70.127	1.00 78.42
545 544		ATOM	4473	OE1	GLU 1	A 56	50	19.960	64.639	69.812	1.00 32.69
# 1000	25	MOTA	4474	OE2	GLU 2	A 56	50	18.593	66.303	70.380	1.00 85.90
1		ATOM	4475	N	GLN 3	A 56	51	16.425	59.627	68.955	1.00 30.45
#= # ₁		ATOM	4476	CA	GLN .			16.467	58.356	68.230	1.00 22.57
igi.		ATOM	4477	С	GLN :	A 56	51	15.398	57.523	68.878	1.00 26.95
		ATOM	4478	0	GLN :	A 56	51	14.978	57.814	69.975	1.00 27.79
27.3	30	ATOM	4479	CB	GLN .	A 56	51	17.829	57.661	68.128	1.00 20.64
		ATOM	4480	CG	GLN .	A 56	51	18.470	57.290	69.491	1.00 22.59
1 100		ATOM	4481	CD	GLN .	A 56	51	17.802	56.121	70.184	1.00 28.22
		MOTA	4482	OE1	GLN :	A 56	51	17.524	56.156	71.400	1.00 37.44
		ATOM	4483	NE2	GLN .	A 56	61	17.556	55.069	69.419	1.00 31.92
ht.	- 35	ATOM	4484	N	GLY .	A 56	62	14.888	56.535	68.209	1.00 26.16
3		ATOM	4485	CA	GLY .	A 56	62	13.801	55.810	68.858	1.00 27.83
		ATOM	4486	С	GLY .	A 56	52	13.932	54.320	68.761	1.00 41.56
		ATOM	4487	0	GLY .	A 56	62	12.936	53.614	68.677	1.00 45.37
		ATOM	4488	N	ARG .			15.171	53.864	68.742	1.00 37.40
	40	MOTA	4489	CA	ARG .			15.457	52.453	68.689	1.00 34.41
		MOTA	4490	C	ARG .	A 56	63	15.121	51.939	70.109	1.00 39.48
		ATOM	4491	0	ARG .			15.832	52.221	71.087	1.00 40.29
		ATOM	4492	CB	ARG			16.932	52.231	68.284	1.00 18.23
		MOTA	4493	CG	ARG			17.309	50.755	68.169	1.00 20.07
	45	MOTA	4494	CD	ARG .			18.779	50.514		1.00 25.07
		MOTA	4495	NE	ARG			19.234	49.139	68.320	1.00 25.66
		MOTA	4496	CZ	ARG			20.425	48.891	67.821	1.00 26.35
		ATOM	4497		AŖG			21.257	49.860	67.430	1.00 12.96
	50	MOTA	4498		ARG			20.804	47.636	67.656	1.00 30.31
	50	MOTA	4499	N	MET			13.989	51.228	70.239	1.00 33.12
		ATOM	4500	CA	MET			13.487	50.695	71.526	1.00 31.84
		ATOM	4501	С	MET			14.565	50.247	72.532	1.00 31.42
**		ATOM	4502	0	MET			14.494	50.501	73.744	1.00 25.72
	EE	ATOM	4503	CB	MET			12.323	49.682	71.365	1.00 32.45
	55	ATOM	4504	CG	MET			11.196	50.225	70.487	1.00 35.78
		ATOM	4505	SD	MET			9.695	49.205	70.533	1.00 40.85
		ATOM	4506	CE	MET			10.177	47.892	69.382	1.00 35.87
		ATOM	4507	N	LYS			15.562	49.581	71.966	1.00 31.68
	(0	MOTA	4508	CA	LYS			16.699	49.041	72.668	1.00 29.04
	60	MOTA	4509	С	LYS			17.281	50.089	73.562	1.00 26.36
		MOTA	4510	0	LYS			17.648	49.782	74.673	1.00 21.19
		MOTA	4511	CB	LYS			17.747	48.494	71.697	1.00 29.06
		MOTA	4512	CG	LYS			18.864	47.715	72.359	1.00 23.89
		ATOM	4513	CD	LYS	A 5	65	19.982	47.355	71.392	1.00 35.75

	ATOM	4514	CE	LYS A 565	20.796	46.153	71.842	1 00	36.31
	ATOM	4515	NZ	LYS A 565			71.577		44.91
	ATOM	4516	N	PHE A 566	17.321		73.073		22.91
1 1	MOTA	4517	CA	PHE A 566			73.833		24.36
5	ATOM	4518	С	PHE A 566			74.571		30.37
	MOTA	4519	0	PHE A 566			75.758		30.52
	ATOM	4520	CB	PHE A 566	18.622		72.857		25.26
	ATOM	4521	CG	PHE A 566			72.088		24.09
	ATOM	4522	CD1	PHE A 566			72.609		23.51
10	ATOM	4523		PHE A 566			70.858		24.48
	MOTA	4524		PHE A 566			71.900		23.73
	MOTA	4525		PHE A 566			70.129		24.75
	ATOM	4526	CZ	PHE A 566			70.668		25.20
	ATOM	4527	N	THR A 567			73.801		31.17
15	ATOM	4528	CA	THR A 567			74.239		31.74
	ATOM	4529	С	THR A 567			75.458		
	MOTA	4530	0	THR A 567		54.818	76.373		
	MOTA	4531	СВ	THR A 567			73.017		26.01
	ATOM	4532		THR A 567		55.844	72.138	1.00	
20	ATOM	4533	CG2						24.12
	ATOM	4534	N	ARG A 568			73.473		34.94
	ATOM	4535	CA	ARG A 568		52,726 52,166	75.469	1.00	30.74
	ATOM	4536	C	ARG A 568			76.545		26.30
	ATOM	4537	ŏ	ARG A 568			77.882		28.61
25	ATOM	4538	СВ	ARG A 568			78.832		30.84
	ATOM	4539	CG	ARG A 568		50.798	76.251		18.11
	ATOM	4540	CD	ARG A 568		50.919	75.088		29.19
	ATOM	4541	NE	ARG A 568		49.660	74.799		19.19
	ATOM	4542	CZ	ARG A 568		49.343	75.917		28.72
30	ATOM	4543		ARG A 568		48.138	76.133		32.39
50	ATOM	4544		ARG A 568		47.144	75.291		29.79
	ATOM	4545	Nnz			47.930	77.208		16.44
	ATOM	4546	CA	PRO A 569 PRO A 569		51.774	77.925		28.41
	ATOM	4547	CA	PRO A 569		51.709	79.154		28.01
35	ATOM	4548	Ö	PRO A 569		53.042	79.663		32.18
55	ATOM	4549	CB	PRO A 569		53.256	80.869		29.25
	ATOM	4550	CG	PRO A 569		50.732	78.919		28.83
	ATOM	4551	CD	PRO A 569		50.034	77.592		32.42
	ATOM	4552	N	LEU A 570		50.829	76.893		29.82
40	ATOM	4553	CA	LEU A 570		53.949	78.741		31.95
	ATOM	4554	C	LEU A 570		55.270	79.160		35.11
	ATOM	4555	0	LEU A 570		55.962	79.897	1.00	36.24
	ATOM	4556	СВ	LEU A 570		56.506	81.028		34.02
	ATOM	4557				56.110	77.932		37.06
45	ATOM	4558	CD1	LEU A 570 LEU A 570	18.387	55.701	77.343		41.39
	ATOM	4559		LEU A 570		56.462	76.050		41.06
	ATOM	4560	N N	PHE A 571	19.497	55.984	78.353		37.42
	ATOM	4561	CA	PHE A 571	14.262	55.944	79.211		30.06
	ATOM	4562	C	PHE A 571	13.084	56.541	79.758		27.27
50	ATOM	4563	o	PHE A 571	12.813	55.899	81.095		25.94
-	ATOM	4564	СВ	PHE A 571	12.399	56.536	82.030		27.16
	ATOM	4565	CG	PHE A 571	11.888	56.375	78.828		27.60
	MOTA	4566		PHE A 571	11.546	57.616	78.042		27.70
	ATOM	4567		PHE A 571	11.193	58.820	78.651		29.97
55	ATOM	4568		PHE A 571	11.557	57.570	76.651		28.87
55					10.861	59.953	77.910		28.24
	ATOM ATOM	4569 4570		PHE A 571	11.233	58.684	75.886		30.43
			CZ	PHE A 571	10.877	59.875	76.520		29.55
	ATOM	4571	N	LYS A 572	13.089	54.618	81.196		22.77
60	ATOM	4572	CA	LYS A 572	12.845	53.946	82.468		25.43
UU	ATOM	4573	C	LYS A 572	13.783	54.425	83.561		34.48
	MOTA	4574	O	LYS A 572	13.351	54.920	84.602		35.11
	MOTA	4575	CB	LYS A 572	12.736	52.428	82.392		26.89
	MOTA	4576	CG	LYS A 572	11.303	51.911	82.326		44.03
	MOTA	4577	CD	LYS A 572	11.219	50.426	81.922	1.00	57.87

		MOTA	4578	CE	LYS A 572	10.975	50.204	80.422	1.00 65.25
		ATOM	4579	NZ	LYS A 572	11.535	48.954	79.850	1.00 61.06
		ATOM	4580	N	ASP A 573	15.074	54.292	83.319	1.00 31.94
		ATOM	4581	CA	ASP A 573	16.032	54.751	84.291	1.00 30.55
	5	ATOM	4582	С	ASP A 573	15.684	56.166	84.712	1.00 32.26
		ATOM	4583	0	ASP A 573	15.693	56.453	85.895	1.00 31.85
		MOTA	4584	CB	ASP A 573	17.453	54.788	83.718	1.00 32.87
		MOTA	4585	CG	ASP A 573	18.051	53.443	83.487	1.00 33.43
		MOTA	4586	OD1	ASP A 573	17.517	52.422	83.853	1.00 29.11
	10	ATOM	4587	OD2	ASP A 573	19.206	53.501	82.864	1.00 35.22
		ATOM	4588	N	LEU A 574	15.387	57.071	83.745	1.00 29.50
		ATOM	4589	CA	LEU A 574	15.062	58.461	84.109	1.00 27.65
		ATOM	4590	С	LEU A 574	13.887	58.577	85.075	1.00 32.88
		MOTA	4591	0	LEU A 574	13.864	59.411	85.962	1.00 31.04
	15	ATOM	4592	CB	LEU A 574	14.844	59.385	82.909	1.00 26.24
		ATOM	4593	CG	LEU A 574	16.068	59.567	82.027	1.00 30.41
		ATOM	4594		LEU A 574	15.644	59.922	80.582	1.00 28.47
44.86		MOTA	4595		LEU A 574		60.659	82.604	1.00 27.06
	20	ATOM	4596	N	ALA A 575		57.723	84.874	1.00 32.80
	20	ATOM	4597	CA	ALA A 575		57.713	85.711	1.00 31.11
ųD		MOTA	4598	С	ALA A 575		57.140	87.083	1.00 35.71
- A		MOTA	4599	0	ALA A 575		57.362	88.055	1.00 39.91
HE PAR		ATOM	4600	CB	ALA A 575		56.890	85.024	1.00 30.56
mågar/ årår	25	ATOM	4601	N	ALA A 576		56.364	87.170	1.00 28.55
UN.	25	ATOM	4602	CA	ALA A 576		55.778	88.448	1.00 22.80
Ped it. B∴n		ATOM	4603	C	ALA A 576		56.724	89.266	1.00 26.93
1		ATOM	4604	0	ALA A 576		56.591	90.461	1.00 30.45
#		MOTA	4605	CB	ALA A 576		54.415 57.686	88.245	1.00 20.31
and the	30	MOTA	4606	N	PHE A 577		58.673	88.584 89.194	1.00 22.86
T.	30	ATOM ATOM	4607 4608	CA C	PHE A 577		59.751	89.673	1.00 22.71 1.00 32.25
		ATOM	4609	Ö	PHE A 577		60.334	88.863	1.00 32.23
ar my		ATOM	4610	CB	PHE A 577		59.188	88.154	1.00 34.17
27 FF		ATOM	4611	CG	PHE A 577		60.076	88.741	1.00 23.16
fin giv	35	· ATOM	4612	CD1			60.231	90.120	1.00 26.60
Sec. and	•	ATOM	4613	CD2			60.806	87.914	1.00 23.46
		ATOM	4614		PHE A 577		61.082	90.661	1.00 27.55
		ATOM	4615	CE2	PHE A 577		61.657	88.431	1.00 23.88
		ATOM	4616	CZ	PHE A 577		61.791	89.813	1.00 23.59
	40	ATOM	4617	N	ASP A 578	14.625	60.008	90.990	1.00 29.70
		MOTA	4618	CA	ASP A 578	13.717	61.018	91.533	1.00 28.65
		MOTA	4619	С	ASP A 578	13.862	62.357	90.881	1.00 28.55
		MOTA	4620	0	ASP A 578	12.877	63.004	90.599	1.00 32.65
		MOTA	4621	CB	ASP A 578	13.804	61.192	93.055	1.00 32.60
	45	MOTA	4622	CG	ASP A 578		61.647	93.550	1.00 53.21
		MOTA	4623		ASP A 578		61.594	92.872	1.00 51.81
		MOTA	4624		ASP A 578		62.072	94.796	1.00 64.93
		MOTA	4625	N	LYS A 579		62.750	90.674	1.00 20.12
	50	MOTA	4626	CA	LYS A 579		64.012	90.084	1.00 21.01
	50	MOTA	4627	С	LYS A 579		64.270	88.697	1.00 30.25
		ATOM	4628	0	LYS A 579			88.368	1.00 35.12
		ATOM	4629	CB	LYS A 579		64.223	90.104	1.00 24.11
		ATOM	4630	CG	LYS A 579			91.512	1.00 48.98
	55	ATOM	4631	CD	LYS A 579			92.286	1.00 76.92
	رر	ATOM	4632	CE	LYS A 579			93.588	1.00 87.93
		ATOM	4633	NZ N	LYS A 579 SER A 580			94.611 87.857	1.00 89.56 1.00 28.66
		ATOM ATOM	4634 4635	n CA				86.459	
		ATOM	4635	C	SER A 580 SER A 580			86.129	1.00 28.56 1.00 32.95
	60	ATOM	4637	0	SER A 580			84.992	1.00 32.93
	50	MOTA	4638	CB	SER A 580			85.517	1.00 25.69
		MOTA	4639	OG	SER A 580			85.969	1.00 25.12
		MOTA	4640	N .	HIS A 58			87.098	1.00 26.81
		ATOM	4641	CA	HIS A 58			86.850	1.00 28.26
		-11 011					0000	0 - 3 0 0 0	

		2 2001	4640	~						
		ATOM	4642	С	HIS A		10.067	62.399	86.042	1.00 36.50
		ATOM	4643	0	HIS A	581	9.644	62.031	84.927	1.00 34.71
		ATOM	4644	СВ	HIS A	581	10.553	61.047	88.152	1.00 29.76
		ATOM	4645	CG	HIS A					
	5						9.148	60.588	87.968	1.00 35.31
	5	ATOM	4646		HIS A		8.111	61.494	87.899	1.00 38.92
		MOTA	4647		HIS A		8.634	59.338	87.891	1.00 36.84
		ATOM	4648	CE1	HIS A	581	6.999	60.783	87.817	1.00 38.85
		MOTA	4649		HIS A		7.280	59.488	87.734	
		ATOM	4650	N	ASP A					1.00 38.13
	10						9.656	63.502	86.639	1.00 35.79
	10	MOTA	4651	CA	ASP A		8.680	64.388	86.064	1.00 34.39
		ATOM	4652	С	ASP A		9.035	64.807	84.659	1.00 37.82
		ATOM	4653	0	ASP A	582	8.220	64.704	83.735	1.00 37.01
		ATOM	4654	CB	ASP A	582	8.428	65.552	87.001	1.00 36.57
		ATOM	4655	CG	ASP A		7.597			
	15	ATOM	4656		ASP A			65.110	88.167	1.00 58.09
	13						6.708	64.289	88.070	1.00 63.17
		ATOM	4657		ASP A		7.920	65.708	89.279	1.00 73.96
		MOTA	4658	N	GLN A	583	10.272	65.255	84.488	1.00 32.88
CJ.		ATOM	4659	CA	GLN A	583	10.750	65.648	83.169	1.00 29.92
20 m/ -		MOTA	4660	С	GLN A	583	10.690	64.464	82.168	1.00 37.12
W.	20	ATOM	4661	0	GLN A		10.362	64.624		
14.5 mg		ATOM	4662	СВ	GLN A				80.990	1.00 37.42
14							12.172	66.182	83.287	1.00 28.54
		MOTA	4663	CG	GLN A		12.704	66.648	81.929	1.00 48.12
		MOTA	4664	CD	GLN A		13.957	67.475	82.081	1.00 64.09
1000 2005		ATOM	4665	OE1	GLN A	583	14.736	67.248	83.015	1.00 59.43
	25	ATOM	4666	NE2			14.130	68.461	81.201	1.00 55.34
1 :		ATOM	4667	N	ALA A		11.009			
h fi		ATOM	4668					63.250	82.638	1.00 33.22
15				CA	ALA A		10.964	62.062	81.780	1.00 32.22
Just.		ATOM	4669	С	ALA A		9.557	61.841	81.315	1.00 37.45
		MOTA	4670	0	ALA A		9.319	61.526	80.152	1.00 40.05
N.	30	ATOM	4671	CB	ALA A	584	11.389	60.793	82.504	1.00 31.62
n.		ATOM	4672	N	VAL A		8.622	61.995	82.261	1.00 30.42
12.0		MOTA	4673	CA	VAL A		7.217			
425 BEV		ATOM	4674	C				61.806	81.946	1.00 29.16
Same of the same o					VAL A		6.647	62.909	81.024	1.00 36.53
- A	25	ATOM	4675	0	VAL A		5.933	62.690	80.052	1.00 36.22
2.0	35	ATOM	4676	CB	VAL A		6.408	61.567	83.209	1.00 29.78
		ATOM	4677	CG1	VAL A	585	4.959	61.947	82.955	1.00 30.03
		ATOM	4678	CG2	VAL A	585	6.464	60.085	83.539	1.00 27.82
		ATOM	4679	N	ARG A		7.000			
		ATOM	4680	CA	ARG A			64.123	81.333	1.00 35.76
	40						6.574	65.242	80.562	1.00 36.20
	40	ATOM	4681	С	ARG A		7.146	65.125	79.180	1.00 44.65
		ATOM	4682	0	ARG A		6.459	65.355	78.197	1.00 48.32
		AŤOM	4683	CB	ARG A	586	7.116	66.498	81.208	1.00 38.13
		ATOM	4684	CG	ARG A	586	6.744	67.799	80.518	1.00 61.01
		ATOM	4685	CD	ARG A		7.077	69.029	81.354	1.00 73.03
	45	ATOM	4686	NE	ARG A		8.491			
		ATOM	4687	CZ				69.128	81.711	1.00 86.05
		ATOM			ARG A		8.961	69.001	82.957	1.00 98.46
			4688		ARG A		8.167	68.741	84.004	1.00 79.75
		ATOM	4689	NH2	ARG A		10.268	69.103	83.159	1.00 77.55
	50	ATOM	4690	N	THR A		8.426	64.769	79.110	1.00 39.49
	50	ATOM	4691	CA	THR A	587	9.099	64.646	77.822	1.00 36.80
		ATOM	4692	С	THR A		8.387	63.690	76.869	
		ATOM	4693	ō	THR A		,			1.00 37.11
		ATOM	4694	СВ			8.229	63.931	75.678	1.00 36.91
					THR A		10.634	64.384	77.917	1.00 39.40
	55	ATOM	4695		THR A		11.303	65.334	78.717	1.00 46.27
	33	ATOM	4696	CG2	THR A		11.233	64.460	76.529	1.00 32.60
		ATOM	4697	N	TYR A	588	7.934	62.587	77.393	1.00 33.33
		ATOM	4698	CA	TYR A		7.252	61.639	76.555	
		ATOM	4699	С	TYR A		5.890			1.00 33.94
		ATOM	4700					62.146	76.090	1.00 37.02
	60			0	TYR A		5.428	61.880	74.988	1.00 41.55
	JV	ATOM	4701		TYR A		7.042	60.383	77.396	1.00 33.96
		MOTA	4702	CG	TYR A		6.017	59.440	76.851	1.00 33.08
		ATOM	4703	CD1	TYR A	588	6.331	58.640	75.754	1.00 35.64
		ATOM	4704		TYR A		4.758	59.288	77.437	1.00 33.04
		ATOM	4705		TYR A		5.424			1 00 34.09
		•		,±)= 	A		J.724	57.703	75.251	1.00 34.36

	ATOM	4706	CE2	TYR A 5	88	3.822	58.378	76.932	1 00	34.05
	ATOM	4707	CZ	TYR A 5		4.162	57.581	75.834		
		4708	OH							33.89
	ATOM			TYR A 5		3.275	56.674	75.322		23.43
	ATOM	4709	N	GLN A 5	89	5.216	62.853	76.959	1.00	25.04
5	MOTA	4710	CA	GLN A 5	89	3.914	63.339	76.612	1.00	21.41
	ATOM	4711	C	GLN A 5	89	3,992	64.304	75.481		28.78
	ATOM	4712	0	GLN A 5		3.099	64.410	74.678		
										31.24
	ATOM	4713	CB	GLN A 5		3.241	63.935	77.832	1.00	21.73
10	ATOM	4714	CG	GLN A 5		2.878	62.820	78.827	1.00	22.30
10	MOTA	4715	CD	GLN A 5	89	1.695	62.069	78.293	1.00	52.83
	MOTA	4716	OE1	GLN A 5	89	1.511	62.003	77.075		60.15
	ATOM	4717	NE2			0.864	61.542	79.182		53.04
	ATOM	4718	N	GLU A 5						
						5.099	65.001	75.409		28.36
15	ATOM	4719	CA	GLU A 5		5.276	65.966	74.355	1.00	26.87
15	ATOM	4720	С	GLU A 5		5.840	65.338	73.140	1.00	35.10
	MOTA	4721	0	GLU A 5	90	6.096	66.059	72.171		40.28
ate in.	ATOM	4722	СВ	GLU A 5		6.323	67.011	74.747		27.61
- en-	ATOM	4723	CG	GLU A 5		5.846				
							67.954	75.847		44.11
20	ATOM	4724	CD	GLU A 5		6.981	68.759	76.388		75.35
	ATOM	4725		GLU A 5		8.120	68.689	75.925	1.00	54.78
je in	MOTA	4726	OE2	GLU A 5	90	6.609	69.516	77.403		59.46
in the second	ATOM	4727	N	HIS A 5	91	6.091	64.031	73.207		27.57
8 445	ATOM	4728	CA	HIS A 5		6.713	63.384	72.086		
ing m/	ATOM	4729	C	HIS A 5						25.58
25						5.928	62.249	71.578		32.34
25	ATOM	4730	0	HIS A 5		6.184	61.751	70.496	1.00	38.53
	ATOM	4731	CB	HIS A 5	91	8.094	62.851	72.487	1.00	26.32
P	MOTA	4732	CG	HIS A 5	91	9.219	63.809	72.268	1.00	31.06
la fin	ATOM	4733	ND1	HIS A 5	91	9.630	64.680	73.255		32.65
n i	MOTA	4734		HIS A 5		9.998	64.032			
30	ATOM	4735						71.169		34.91
20				HIS A 5		10.635	65.404	72.756		32.01
	ATOM	4736		HIS A 5		10.884	65.037	71.508	1.00	33.36
L1	ATOM	4737	N	LYS A 5	92	4.978	61.812	72.337	1.00	28.34
	ATOM	4738	CA	LYS A 5	92	4.254	60.643	71.849		29.96
in the	ATOM	4739	С	LYS A 5		3.654	60.692	70.432		33.41
35	ATOM	4740	Ō	LYS A 5			59.769			
7.7						3.819		69.592		29.05
	ATOM	4741	СВ	LYS A-5		3.362	59.983	72.888		32.83
	ATOM	4742	CG	LYS A 5		2.435	60.930	73.615	1.00	31.14
	ATOM	4743	CD	LYS A 5	92	1.677	60.203	74.704	1.00	38.97
	ATOM	4744	CE	LYS A 5	92	0.253	60.691	74.890		25.02
40	ATOM	4745	NZ	LYS A 5	92	-0.157	60.632	76.302		45.83
	ATOM	4746	N	ALA A 5		2.934	61.782			
	ATOM	4747	CA	ALA A 5				70.187		30.97
						2.260	62.026	68.917		28.47
	ATOM	4748	С	ALA A 5		3.169	61.943	67.703	1.00	32.66
4.5	ATOM	4749	0	ALA A 5		2.775	61.488	66 .6 39	1.00	36.77
45	ATOM	4750	CB	ALA A 5	93	1.571	63.379	68.954	1.00	27.35
	MOTA	4751	N	SER A 5	94	4.384	62.405	67.869		27.08
	ATOM	4752	CA	SER A 5		5.345	62.417	66.794		30.04
	ATOM	4753	C	SER A 5						
	ATOM	4754				6.185	61.169	66.760		36.80
50			0	SER A 5		6.995	60.991	65.848		37.94
50	ATOM	4755	CB	SER A 5		6.292	63.596	66.977	1.00	37.69
	MOTA	4756	OG	SER A 5	94	7.199	63.340	68.043	1.00	54.55
	MOTA	4757	N	MET A 5	95	6.015	60.340	67.776		33.12
	MOTA	4758	CA	MET A 5		6.794	59.115	67.898		33.96
	ATOM	4759	c	MET A 5						
55						6.200	57.936	67.125		40.91
J.J.	ATOM	4760	0	MET A 5		5.019	57.927	66.809		50.82
	ATOM	4761	CB	MET A 5		6.716	58.686	69.382	1.00	34.22
	ATOM	4762	CG	MET A 5	95	7.621	59.371	70.399		34.61
	MOTA	4763	SD	MET A 5		7.606	58.440	71.962		39.24
	ATOM	4764	CE	MET A 5						
60	ATOM	4765				7.145	59.779	73.084		36.72
55			N	HIS A 5		6.987	56.897	66.886		26.19
	ATOM	4766	CA	HIS A 5		6.496	55.657	66.246	1.00	23.19
	ATOM	4767	С	HIS A 5		5.438	54.964	67.120		25.21
	MOTA	4768	0	HIS A 5		5.621	54.728	68.311		22.59
	MOTA	4769	CB	HIS A 5	96	7.657	54.655	66.077		24.41
										7

WO 00/50577

		4330	~~	****	500		2 000	50 000	CC 400	
	MOTA	4770	CG	HIS A			7.222	53.366	65.493	1.00 30.13
	MOTA	4771		HIS A			7.606	52.995	64.214	1.00 32.86
	MOTA	4772	CD2	HIS A	596		6.421	52.385	66.005	1.00 30.90
	ATOM	4773	CE1	HIS A	596		7.047	51.824	63.974	1.00 30.05
5	ATOM	4774	NE2	HIS A	596		6.325	51.441	65.031	1.00 30.20
	ATOM	4775	N	PRO A			4.334	54.587	66.512	1.00 27.08
		4776	CA		597				67.173	
	MOTA					•	3.217	53.912		1.00 26.35
	MOTA	4777	C	PRO A			3.513	52.851	68.248	1.00 37.51
	MOTA	4778	0	PRO A	597		2.979	52.900	69.348	1.00 41.16
10	ATOM	4779	CB	PRO P	597		2.334	53.307	66.076	1.00 26.17
	A.TOM	4780	CG	PRO A	597		3.140	53.426	64.792	1.00 34.56
	ATOM	4781	CD	PRO A	597		4.285	54.418	65.050	1.00 30.06
	ATOM	4782	N	VAL A			4.311	51.850	67.939	1.00 33.08
	ATOM	4783	CA	VAL A			4.585	50.802	68.911	
15										1.00 28.39
13	MOTA	4784	С	VAL A			5.444	51.307	70.029	1.00 29.32
	MOTA	4785	0	VAL A			5.168	51.096	71.217	1.00 29.13
	MOTA	4786	CB	VAL A			5.196	49.599	68.210	1.00 27.99
	MOTA	4787	CG1	VAL A	1 598		5.806	48.608	69.187	1.00 26.98
车辆 。	MOTA	4788	CG2	VAL A	1 598		4.144	48.944	67.296	1.00 26.13
20	ATOM	4789	N	THR A	599		6.480	52.021	69.635	1.00 26.10
	ATOM	4790	CA	THR A			7.370	52.573	70.631	1.00 26.95
	ATOM	4791	C	THR A			6.650			
in An								53.404	71.669	1.00 30.81
新来	ATOM	4792	0	THR A			6.863	53.327	72.871	1.00 31.33
र्हे म र	ATOM	4793	CB	THR A			8.413	53.455	69.975	1.00 26.67
25	MOTA	4794		THR A			9.092	52.725	68.958	1.00 27.92
15	MOTA	4795	CG2	THR A	A 599		9.358	53.884	71.092	1.00 20.69
50 W.	MOTA	4796	N	ALA A	4 600		5.801	54.218	71.135	1.00 26.41
4	MOTA	4797	CA	ALA A			4.997	55.111	71.878	1.00 26.39
4	ATOM	4798	C	ALA A			4.176	54.339	72.860	1.00 32.00
30		4799	Ö	ALA A						
7. Ju	ATOM						4.162	54.597	74.057	1.00 35.37
5 m2	MOTA	4800	CB	ALA A			4.090	55.774	70.856	1.00 27.56
MJ	ATOM	4801	N	MET A			3.470	53.380	72.332	1.00 26.26
13	ATOM	4802	CA	MET A			2.627	52.585	73.167	1.00 26.60
F7.	MOTA	-4803	C	MET 2	4 601		3.439	51.909	74.225	1.00 25.73
35	ATOM	4804	0	MET A	A 601		3.099	51.964	75.381	1.00 25.77
15 m	ATOM	4805	CB	MET A	A 601		1.752	51.625	72.353	1.00 30.49
	ATOM	4806	CG	MET A	A 601		1.024	50.594	73.176	1.00 36.00
	ATOM	4807	SD	MET A			2.043	49.146	73.554	1.00 42.41
	ATOM	4808	CE	MET A			1.693	48.128	72.111	1.00 37.75
40	ATOM	4809	N	LEU A			4.538	51.310	73.848	1.00 37.73
		4810	CA	LEU A			5.339			
	ATOM			LEU I				50.671	74.873	1.00 22.59
	ATOM	4811	C				6.010	51.650	75.870	1.00 29.61
	ATOM	4812	0	LEU A			6.137	51.346	77.039	1.00 27.62
4.5	ATOM	4813	CB	LEU 2			6.418	49.760	74.294	1.00 22.14
45	MOTA	4814	CG	LEU A	A 602		5.916	48.529	73.575	1.00 25.78
	MOTA	4815	CD1	LEU A	A 602		7.021	48.087	72.609	1.00 26.02
	MOTA	4816	CD2	LEU A	A 602		5.651	47.445	74.613	1.00 21.01
	ATOM	4817	N	VAL A	A 603		6.508	52.805	75.445	1.00 27.15
	ATOM	4818	CA		A 603		7.145	53.684	76.413	1.00 26.39
50	ATOM	4819	c		A 603		6.121	54.157	77.438	
20	ATOM	4820	Ö							1.00 32.60
					A 603		6.436	54.235	78.621	1.00 35.31
	ATOM	4821	CB		A 603		7.917	54.832	75.760	1.00 27.78
	ATOM	4822		VAL 3			8.286	55.887	76 .774	1.00 24.54
	MOTA	4823	CG2	VAL 2			9.172	54.286	75.094	1.00 27.29
55	ATOM	4824	N		A 604		4.878	54.434	76.976	1.00 27.44
	ATOM	4825	CA	GLY Z	A 604		3.759	54.856	77.819	1.00 27.58
	ATOM	4826	С		A 604		3.418	53.797	78.905	1.00 37.00
	ATOM	4827	ō		A 604		3.088	54.102	80.072	1.00 36.56
	ATOM	4828	N		A 605		3.511	52.522	78.520	
60										1.00 32.54
· · · · ·	ATOM	4829	CA		A 605		3.250	51.415	79.459	1.00 32.17
	ATOM	4830	C		A 605		4.312	51.405	80.539	1.00 35.15
	ATOM	4831	0		A 605		4.040	51.347	81.734	1.00 33.77
	MOTA	4832	CB		A 605		3.231	50.034	78.782	1.00 33.59
	ATOM	4833	CG	LYS I	A 605		1.837	49.438	78.576	1.00 42.45

PCT/SE00/00384 WO 00/50577

	MOTA	4834	CD	LYS	Α	605	1.	846	48.115	77.815	1.00 60.83
	MOTA	4835	CE	LYS				223	46.946	78.578	1.00 86.38
	ATOM	4836	NZ	LYS				188	46.179	79.385	1.00 93.05
	ATOM	4837		ASP				544	51.470	80.056	1.00 32.91
5	ATOM	4838		ASP				715	51.510	80.878	1.00 31.82
	ATOM	4839		ASP				549	52.667	81.833	1.00 36.24
	ATOM	4840		ASP				652	52.503	83.045	1.00 35.19
	MOTA	4841		ASP				983	51.702	80.027	1.00 32.52
10	ATOM	4842	CG	ASP				302	50.525	79.134	1.00 40.01
10	ATOM	4843		ASP				934	49.378	79.344	1.00 40.49
	ATOM	4844		ASP LEU				038	50.869	78.111	1.00 41.73
	ATOM ATOM	4845 4846	N CA	LEU				240	53.833	81.266	1.00 34.45
	ATOM	4847	CA	LEU				152	54.972 55.018	82.185 82.968	1.00 36.03
15	ATOM	4848	Õ	LEU				814 600	55.872	83.824	1.00 42.35
15	ATOM	4849	СВ	LEU				321	56.250	81.364	1.00 41.57 1.00 36.90
	ATOM	4850	CG	LEU				779	56.490	80.974	1.00 38.75
	ATOM	4851		LEU				954	57.746	80.132	1.00 34.34
C9	ATOM	4852		LEU				695	56.653	82.183	1.00 34.34
20	ATOM	4853	N	LYS				895	54.062	82.586	1.00 45.01
- Table - C	ATOM	4854	CA	LYS				576	53.874	83.264	1.00 46.99
	ATOM	4855	С	LYS				625	55.088	83.181	1.00 51.31
ja ik	ATOM	4856	0	LYS				988	55.467	84.151	1.00 51.35
ing int	ATOM	4857	CB	LYS				813	53.510	84.750	1.00 50.83
25	ATOM	4858	CG	LYS	Α	608	3.	.331	52.093	84.949	1.00 63.57
LT.	ATOM	4859	CD	LYS				405	52.019	86.031	1.00 77.03
}=4x	MOTA	4860	CE	LYS	Α	608		.341	50.825	85.858	1.00 96.40
R	ATOM	4861	NZ	LYS	Α	608	6	.034	50.554	87.117	1.00100.00
1.4.	MOTA	4862	N	VAL	Α	609	1.	.560	55.724	81.991	1.00 50.28
30	MOTA	4863	CA	VAL				.688	56.901	81.852	1.00 50.89
	MOTA	4864	С	VAL				.494	56.660	80.897	1.00 60.23
# # P	ATOM	4865	0	VAL				.640	56.952	81.194	1.00 63.02
# 10 m	ATOM	4866	CB	VAL				.533	58.091	81.364	1.00 54.72
25	MOTA	4867		VAL				.996	58.926	82.551	1.00 54.87
35	ATOM	4868		VAL				.744	57.607	80.605	1.00 54.46
	MOTA MOTA	4869 4870	N CA	ASP ASP			-0	.177 .238	56.152 55.949	79.687 78.699	1.00 58.84
	ATOM	4871	C	ASP				.062	54.695	79.001	1.00 99.84 1.00100.00
	ATOM	4872	õ	ASP				.247	54.615	78.711	1.00 69.75
40	ATOM	4873	СВ	ASP				.594	55.818	77.316	1.00100.00
	ATOM	4874	CG	ASP				.637	57.161	76.610	1.00 92.61
	ATOM	4875		ASP				.449	57.999	77.018	1.00 90.49
	MOTA	4876		ASP				.134	57.355	75.670	1.00 89.29
	ATOM	4877	ZN2+	ZN	Z	1		.003	38.803	64.180	1.00 28.37
45	ATOM	4878	YB3+	YB	Y	1	43	.011	51.068	98.864	1.00 34.70
	ATOM		YB3+		Y	2		.786	56.771	52.040	0.50 57.25
	ATOM		YB3+		Y	3		.537	57.860	52.381	0.50 36.57
	ATOM	4881	CG	IMD		1		.249	42.039	80.754	1.00 28.44
50	ATOM	4882		IMD		1		.057	42.254	79.400	1.00 28.35
50	MOTA	4883		IMD		1		.562	41.726	80.902	1.00 17.99
	MOTA	4884		IMD		1		.201	42.063	78.760	1.00 29.77
	MOTA	4885		IMD		1		.130	41.745	79.647	1.00 35.02
	ATOM ATOM	4886 4887	CB CG	ACE ACE		1 1		.616	12.333	68.475	1.00 59.33
55	ATOM	4888		ACE		1		.871 .958	13.331 14.536	69.306 69.146	1.00 42.98 1.00 39.66
23	ATOM	4889		ACE		1		.142	12.759	70.236	1.00 39.00
	MOTA	4890	C6	INH		ī		.422	38.514	70.154	1.00 38.70
	ATOM	4891	C5	INH		1		.571	39.820	69.689	1.00 37.05
	ATOM	4892	C4	INH		ī		.901	40.062	68.354	1.00 37.03
60	ATOM	4893	C3	INH		1		.091	38.967	67.505	1.00 35.48
	ATOM	4894	C2	INH				.944	37.650	67.949	1.00 31.90
	ATOM	4895	Cl	INH				.611	37.434	69.286	1.00 36.93
	MOTA	4896	c7	INH		1	8	.071	41.463	67.833	1.00 32.28
	MOTA	4897	-01	INH	V	1	8	.288	41.443	66.485	1.00 37.06

	MOTA	4898	C8	INH V	1	9.584	41.740	66.129	1.00 32.34
	ATOM	4899	C9	INH V	1	9.825	42.911	65.416	1.00 31.03
	ATOM	4900		INH V	1	11.127	43.216	65.023	1.00 33.64
_	ATOM	4901		INH V	1	12.194	42.381	65.339	1.00 31.88
5	ATOM	4902		INH V	1	11.928	41.198	66.028	1.00 31.07
	ATOM	4903		INH V	1	10.630	40.858	66.412	1.00 28.70
	ATOM	4904		INH V	1	13.587	42.710	64.882	1.00 32.51
	MOTA	4905		INH V	1	14.260	41.560	64.121	1.00 34.69
10	ATOM	4906		INH V	1	15.683	41.849	63.754	1.00 28.88
10	ATOM	4907	S1	INH V	1	16.605	40.755	64.790	1.00 29.16
	ATOM	4908	N1	INH V	1	13.497	40.805	63.099	1.00 30.69
	ATOM	4909	0	HOH W	1	44.463	49.888	77.523	1.00 46.91
	ATOM	4910		HOH W	2	13.469	27.803	78.018	1.00 20.07
15	ATOM	4911 4912	0	HOH W	3	4.225	69.721	58.393	1.00 27.76
13	MOTA MOTA	4913	0	HOH W	4	15.603	28.826	61.823	1.00 22.81
	ATOM	4913	0	HOH W	5 6	22.862	26.624	42.874	1.00 53.05
	ATOM	4915	0	HOH W	7	8.423	46.452	57.584	1.00 32.22
	ATOM	4916	Ö	HOH W	8	17.904 22.979	46.550	68.524	1.00 31.91
20	ATOM	4917	Ö	HOH W	9	17.707	45.895	83.716	1.00 39.37
43	ATOM	4918	Ö	HOH W	10	12.439	39.158 36.303	55.643	1.00 25.27
j.k.	ATOM	4919	Ö	HOH W	11	17.367	62.730	59.209	1.00 31.46
1 FR: 11 S FR:	ATOM	4920	ŏ	HOH W	12	42.823	52.642	50.320 90.552	1.00 37.74
2 8673	ATOM	4921	Ö	HOH W	13	34.337	45.508	97.419	1.00 53.80 1.00 57.99
25	ATOM	4922	Õ	HOH W	14	6.726	27.119	48.459	1.00 57.99
194 A	ATOM	4923	0	HOH W	15	-0.093	30.159	71.746	1.00 02.29
1-10	ATOM	4924	0	HOH W	16	-19.673	44.016	58.682	1.00 29.96
##	MOTA	4925	0	HOH W	17	16.563	26.790	80.837	1.00 38.62
J=4.	ATOM	4926	0	HOH W	18	10.281	35.677	88.518	1.00 26.01
30	ATOM	4927	0	HOH W	19	20.973	35.691	44.774	1.00 49.50
	ATOM	4928	0	HOH W	20	0.996	19.571	53.713	1.00 67.39
	MOTA	4929	0	HOH W	21	20.424	37.014	85.845	1.00 39.54
	ATOM	4930	0	HOH W	22	-2.498	35.905	53.781	1.00 51.70
4	ATOM	4931	0	HOH W	23	39.807	49.718	92.595	1.00 37.39
35	ATOM	4932	0	HOH W	24	16.431	58.267	93.127	1.00 47.45
	ATOM	4933	0	HOH W	25	6.935	45.104	66.012	1.00 18.12
	ATOM	4934	0	HOH W.		40.479	54.713		1.00 28.72
	ATOM	4935	0	HOH W	27	22.369	40.324	67.919	1.00 46.36
40	ATOM ATOM	4936 4937	0	HOH W	28	37.289	49.457	68.016	1.00 61.37
40	ATOM	4937	0	HOH W	29 30	2.611	35.015	55.709	1.00 24.45
	ATOM	4939	0	HOH W	31	41.088	62.590	98.644	1.00 65.38
	ATOM	4940	0	HOH W	32	17.369 25.433	55.024	87.465	1.00 24.22
	ATOM	4941	ŏ	HOH W	33	3.890	20.198 42.770	55.692	1.00 44.61
45	ATOM	4942	ō	HOH W	34	3.934	63.391	66.651 62.592	1.00 22.34
	ATOM	4943	Ō	HOH W	35	22.280	41.610	86.289	1.00 60.69 1.00 74.20
	ATOM	4944	0	HOH W	36	22.631	46.401	90.078	1.00 47.44
	ATOM	4945	0	HOH W	37	33.442	20.227	64.569	1.00 47.44
	ATOM	4946	0	HOH W	38	39.834	28.974	75.602	1.00 41.72
50	ATOM	4947	0	HOH W	39	35.232	47.140	54.186	1.00 37.08
	ATOM	4948	0	HOH W	40	36.003	57.784	57.893	1.00 43.05
	ATOM	4949	0	HOH W	41	37.216	27.438	74.564	1.00 50.79
	ATOM	4950	0	HOH W	42	17.770	67.012	77.183	1.00 45.78
55	ATOM	4951	0	HOH W	43	5.341	31.286	78.127	1.00 25.34
55	ATOM	4952	0	HOH W	44	33.535	32.503	52.063	1.00 56.13
	ATOM	4953	0	HOH W	45	25.477	33.146	44.610	1.00 65.43
	ATOM	4954	0	HOH W	46	16.235	37.438	52.628	1.00 32.10
	ATOM	4955	0	HOH W	47	28.791	14.101	63.316	1.00 46.67
60	ATOM	4956	0	HOH W	48	10.230	24.992	86.967	1.00 38.63
UU	ATOM	4957	0	HOH W	49	30.821	38.856	79.630	1.00 40.44
	ATOM ATOM	4958 4959	0	HOH W	50	12.621	37.226	62.944	1.00 26.70
	ATOM	4959	0	HOH W	51	27.987	30.609	66.612	1.00 33.55
	ATOM	4961	0	HOH W	52 53	34.459	28.696	64.242	1.00 51.01
		1001	0	.1011 84	J J	34.969	62.270	91.179	1.00 68.20

		4000	_								
	MOTA	4962	0	HOH W	54		33.631	30.717	62.396	1.00	41.64
	ATOM	4963	0	HOH W	55		43.987	48.530	91.269		50.99
	MOTA	4964	0	нон w	56		23.412	28.584	85.186		69.23
	ATOM	4965	0	HOH W			39.834				
5								28.057	72.257		81.00
,	ATOM	4966	0	HOH W			2.892	25.685	69.907	1.00	38.96
	MOTA	4967	0	HOH W	59		10.284	47.120	72.671	1.00	40.28
	ATOM	4968	0	HOH W	60	•	32.645	39.037	76.746		21.71
	ATOM	4969	0	HOH W	61		43.535	48.019	95.228		
	ATOM	4970	ŏ	HOH W							37,69
10					62		11.991	51.053	43.479		41.05
10	ATOM	4971	0	HOH W	63		18.329	56.527	89.388	1.00	28.51
	ATOM	4972	0	HOH W	64		16.555	9.309	68.875	1.00	89.05
	ATOM	4973	0	HOH W	65		23.741	44.759	73.150		38.43
	ATOM	4974	0	нон w	66		19.093	53.805	41.239		
	ATOM	4975	ō	нон w	67						55.25
15		4976					31.750	60.369	56.933		92.26
13	ATOM		0	HOH W	68		24.836	68.428	80.926		59.25
	ATOM	4977	0	HOH W	69		-21.014	19.446	48.342	1.00	52.24
	MOTA	4978	0	HOH W	70		11.318	68.028	86.566		77.81
an en.	ATOM	4979	0	HOH W	71		5.312	60.076	63.511		36.83
	ATOM	4980	0	HOH W	72		7.689	20.219			
20	ATOM								84.680		32.24
40		4981	0	HOH W	73		34.988	44.708	64.746	1.00	40.73
	MOTA	4982	0	HOH W	74		10.614	49.644	41.337	1.00	38.90
jad.	MOTA	4983	0	HOH W	75		19.349	42.973	64.739		54.53
· · · · · · · · · · · · · · · · · · ·	MOTA	4984	0	HOH W	76		35.916	30.862	80.753		55.38
25	ATOM	4985	0	HOH W	77		9.666	26.046			
1 25	ATOM	4986							46.603		40.09
U1 23			0	HOH W	78		-10.171	46.751	60.237	1.00	29.78
j .a.	MOTA	4987	0	HOH W	79		46.751	58.883	86.875	1.00	35.92
	MOTA	4988	0	HOH W	80		19.320	32.528	51.000	1.00	33.36
#	ATOM	4989	0	HOH W	81		28.815	39.568	66.176		59.19
} =4.	ATOM	4990	0	HOH W	82		38.207	35.773	73.585		17.81
1.30	ATOM	4991	ō	HOH W	83						
							23.802	33.925	75.175		25.19
n.	ATOM	4992	0	HOH W	84		42.241	51.290	99.896	1.00	15.88
	ATOM	4993	0	HOH W	85		3.751	36.678	58.842	1.00	24.97
he all	ATOM	4994	0	HOH W	86		-7.009	40.341	62.580		25.39
	ATOM	4995	0	HOH W	87		11.735	58.910	68.155		39.70
35	ATOM	4996	0	HOH W	88		13.986	52.835	42.224		
	ATOM	4997	ŏ	HOH W	89						50.91
							1.452	46.541	69.459		35.03
	MOTA	4998	0	HOH W	90		-1.938	55.310	56.971	1.00	28.10
	MOTA	4999	0	HOH W	91		13.801	66.947	52.600	1.00	38.65
4.0	MOTA	5000	0	HOH W	92		21.594	47.218	79.203		30.31
40	ATOM	5001	0	HOH W	93		10.639	58.632	90.827		43.78
	ATOM	5002	0	HOH W	94		33.335	53.550			
	ATOM	5003	Ö	HOH W	95				68.086		37.04
							-1.984	28.738	60.212		31.56
	ATOM	5004	0	HOH W	96		-4.958	51.055	59.250	1.00	34.00
AE	MOTA	5005	0	HOH W	97		17.610	39.701	51.503	1.00	28.27
45	ATOM	5006	0	HOH W	98		10.686	54.166	67.565		37.68
	ATOM	5007	0	HOH W	99		20.567	43.859	78.621		41.57
	ATOM	5008	0	HOH W			7.013	22.332	69.109		
	ATOM	5009	ō	HOH W							28.72
							10.097	53.225	78.477		35.68
50	MOTA	5010	0	HOH W			10.849	31.404	53.014	1.00	32.22
20	MOTA	5011	0	HOH W			42.381	59.035	94.728	1.00	36.00
	MOTA	5012	0	HOH W	104		17.234	41.111	54.082		33.65
	ATOM	5013	0	HOH W	105		26.902	62.025	81.989		34.70
	ATOM	5014	0	HOH W			-14.313	49.559			
	ATOM	5015	Ö	HOH W					56.204		54.36
55							41.646		101.015		68.12
, 55	ATOM	5016	0	HOH W			26.759	43.000	47.219	1.00	32.69
	ATOM	5017	0	HOH W			16.624	48.119	46.545		38.64
	ATOM	5018	0	HOH W	110		26.159	32.793	75.230		24.77
	MOTA	5019	0	нон w			2.101	33.468	67.006		
	ATOM	5020	ŏ	HOH W							31.50
60							38.114	36.374	87.451		44.06
U.	MOTA	5021	0	HOH W			13.211	29.810	61.356		33.81
	ATOM	5022	0	HOH W			-3.064	37.86 3	40.673	1.00	37.92
	ATOM	5023	0	HOH W			15.007	47.948	69.488		28.23
	MOTA	5024	0	HOH W			27.101	66.633	80.518		41.24
	ATOM	5025	0	HOH W			11.870	38.304	43.174	1 00	40.85
								20.204	30.114	1.00	40.02

WO 00/50577

		MOTA	5026	0	HOH W 118	-13.844	25.597	58.258	1.00 53.75
		ATOM	5027	0	HOH W 119	2.929	41.135	59.858	1.00 36.49
		ATOM	5028	0	HOH W 120	24.890	45.490	82.167	1.00 41.65
		ATOM	5029	0	HOH W 121	36.062	59.335	75.090	1.00 38.82
	5	ATOM	5030	0	HOH W 122	-10.715	32.037	61.699	1.00 78.82
		ATOM	5031	0	HOH W 123	-2.646	25.492	60.812	1.00 48.40
		MOTA	5032	0	HOH W 124	-8.948	46.831	63.556	1.00 48.06
		ATOM	5033	0	HOH W 125	-17.843	39.367	36.020	1.00 35.80
		ATOM	5034	0	HOH W 126	2.218	57.766	62.253	1.00 44.61
	10	ATOM	5035	0	HOH W 127	10.736	62.766	64.366	1.00 55.84
		A'TOM	5036	0	HOH W 128	0.884	35.562	63.963	1.00 44.14
		ATOM	5037	0	HOH W 129	19.165	59.557	60.644	1.00 47.82
		ATOM	5038	0	HOH W 130	1.546	27.875	68.443	1.00 39.69
		MOTA	5039	0	HOH W 131	5.497	26.285	76.668	1.00 44.47
	15	MOTA	5040	0	HOH W 132	14.505	36.538	88.996	1.00 40.00
		MOTA	5041	0	HOH W 133	.8.534	28.713	88.519	1.00 46.55
		MOTA	5042	0	HOH W 134	6.125	45.267	77.959	1.00 45.57
		ATOM	5043	0	HOH W 135	26.016	18.543	78.878	1.00 51.65
		ATOM	5044	0	HOH W 136	33.880	23.025	70.739	1.00 46.95
1	20	MOTA	5045	0	HOH W 137	19.230	26.073	49.998	1.00 51.97
	- L	ATOM	5046	0	HOH W 138	41.563	41.085	77.326	1.00 43.14
i.a.	4.60	ATOM	5047	0	HOH W 139	39.187	63.067	75.380	1.00 56.52
		MOTA	5048	0	HOH W 140	26.878	54.491	67.203	1.00 42.14
SALV.		ATOM	5049	0	HOH W 141	22.988	62.189	74.174	1.00 48.31
15 TO 15 TO 15	25	ATOM	5050	0	HOH W 142	25.190	62.803	71.067	1.00 67.16
U		ATOM	5051	0	HOH W 143	18.598	45.126	81.949	1.00 53.80
=4		ATOM	5052	0	HOH W 144	19.782	53.129	90.556	1.00 48.73
15		MOTA	5053	0	HOH W 145	21.735	48.367	86.454	1.00 40.39
		MOTA	5054	0	HOH W 146	25.707	57.012	93.476	1.00 53.61
	30	ATOM	5055	0	HOH W 147	22.832	62.085	93.149	1.00 46.02
		MOTA	5056	0	HOH W 148	25.725	67.203	89.990	1.00 75.23
# 188 ¹ ## #8.		MOTA	5057	0	HOH W 149	10.773	53.653	85.697	1.00 50.65
25 H		ATOM	5058	0	HOH W 150	4.221	58.449	86.608	1.00 49.23
	2	MOTA	5059	0	HOH W 151	7.790	72.096	84.410	1.00 51.10
- A	35	ATOM	5060	0	HOH W 152	2.387	58.282	6 7.8 35	1.00 33.29
, ,		MOTA	5061	0	HOH W 153	0.921	49.551	69.095	1.00 59.60
		MOTA	5062	0	HOH W 154	8.722	45.171	71.561	1.00 46.56
		MOTA	5063	0	HOH W 155	6.422	47.947	81.081	1.00 57.56
	40	MOTA	5064	0	HOH W 156	15.936	56.908	55.129	1.00 43.33
	40	ATOM	5065	0	HOH W 157	3.032	19.635	62.453	1.00 80.38
		ATOM	5066	0	HOH W 158	-4.228	58.058	47.057	1.00 39.66
		MOTA	5067	0	HOH W 159	1.197	41.002	78.942	1.00 57.22
		ATOM	5068	0	HOH W 160	1.259	43.651	68.100	1.00 37.94
	45	ATOM	5069	0	HOH W 161	25.799	64.833	56.690	1.00 38.96
	43	ATOM	5070	0	HOH W 162	-11.853	45.054	45.070	1.00 38.38
		ATOM	5071 5072	0	HOH W 163 HOH W 164	40.159	31.033	78.548	1.00 75.36
		ATOM	5072	0	HOH W 165	21.477 26.347	20.377	79.349 72.803	1.00 35.96 1.00 42.21
		ATOM ATOM	5074	0	HOH W 166	16.446	44.558 61.207	59.687	1.00 42.21
	50	ATOM	5075	0	HOH W 167	27.695	64.216	82.410	1.00 39.70
	20	ATOM	5076	0	HOH W 168	-2.998	57.511	34.738	1.00 45.35
		ATOM	5077	ŏ	HOH W 169	6.608	51.527	60.826	1.00 43.33
		ATOM	5078	Ö	HOH W 170	31.104	28.934	81.337	1.00 43.19
		ATOM	5079	Ö	HOH W 171	10.135	28.233	45.533	1.00 41.24
	55	ATOM	5080	Ö	HOH W 172	8.201	43.960	75.322	1.00 37.71
	23	ATOM	5081	Ö	HOH W 173	13.799	66.601	85.597	1.00 37.71
		ATOM	5082	0	HOH W 174	16.664	53.670	65.006	1.00 34.74
		MOTA	5083	Ö	HOH W 175	18.301	47.296	43.793	1.00 45.84
		ATOM	5084	ő	HOH W 176	11.717	61.868	52.648	1.00 45.84
	60	ATOM	5085	Ö	HOH W 177	29.516	23.822	76.838	1.00 51.50
		MOTA	5086	ŏ	HOH W 178	39.940	60.509	78.535	1.00 46.33
		ATOM	5087	ō	HOH W 179	-1.803	44.974	37.278	1.00 52.56
		ATOM	5088	ō	HOH W 180	7.343	47.305	65.468	1.00 47.27
		ATOM	5089	ō	HOH W 181	17.912	15.338	81.793	1.00 50.08

	ATOM	5090	0	HOH W 182	-4.631	55.917	82.183	1.00 65.36
	ATOM	5091	ō	HOH W 183	32.973	42.656	86.667	1.00 43.97
	ATOM	5092	ō	HOH W 184	-1.834	36.784	71.040	1.00 45.10
	ATOM	5093	ō	HOH W 185	-4.519	34.633	71.838	1.00 43.10
5	ATOM	5094	ŏ	HOH W 186	4.518	68.554	71.661	1.00 46.99
J		5095	o	HOH W 187	2.774			
	ATOM	5095	0	HOH W 187	31.770	37.503	61.490	1.00 45.81
	ATOM					43.526	51.410	1.00 58.02
	ATOM	5097	0	HOH W 189	5.471	43.861	38.891	1.00 49.43
10	ATOM	5098	0	HOH W 190	11.934	58.219	70.811	1.00 49.96
10	ATOM	5099	0	HOH W 191	33.112	26.203	70.484	1.00 60.03
	MOTA	5100	0	HOH W 192	30.914	43.017	70.613	1.00 73.23
	MOTA	5101	0	HOH W 193	0.400	39.300	39.714	1.00 65.37
	MOTA	5102	0	HOH W 194	48.247	56.159	86.370	1.00 60.09
15	MOTA	5103	0	HOH W 195	12.359	59.992	62.698	1.00 53.57
15	MOTA	5104	0	HOH W 196	11.149	17.504	78.264	1.00 54.43
	ATOM	5105	0	HOH W 197	-4.284	31.953	60.991	1.00 47.12
	ATOM	5106	0	HOH W 198	29.888	35.624	82.772	1.00 52.16
	MOTA	5107	0	HOH W 199	14.388	39.115	89.656	1.00 47.93
	ATOM	5108	0	HOH W 200	-8.529	51.475	47.745	1.00 61.00
20	ATOM	5109	0	HOH W 201	-15.572	53.338	52.008	1.00 72.42
	ATOM	5110	0	HOH W 202	24.319	38.590	87.128	1.00 50.03
14 da	ATOM	5111	Ο,	HOH W 203	25.366	70.670	82.839	1.00 49.01
2 m	ATOM	5112	0	HOH W 204	18.531	27.749	86.236	1.00 48.64
	ATOM	5113	0	HOH W 205	21.694	20.030	81.796	1.00 49.04
25	ATOM	5114	0	HOH W 206	23.953	47.993	67.580	1.00 40.39
17	ATOM	5115	0	HOH W 207	22.012	40.217	90.228	1.00 42.29
j=4.	ATOM	5116	0	HOH W 208	16.197	45.094	43.427	1.00 48.00
	ATOM	5117	0	HOH W 209	21.019	68.985	84.382	1.00 56.50
# *	ATOM	5118	ō	HOH W 210	-7.134	33.015	71.591	1.00 56.31
30	ATOM	5119	ō	HOH W 211	40.843	44.050	89.284	1.00 43.07
	ATOM	5120	ō	HOH W 212	20.374	14.856	56.642	1.00 50.07
T.	ATOM	5121	ō	HOH W 213	12.723	46.277	73.748	1.00 59.15
C)	MOTA	5122	o	HOH W 214	8.956	43.704	58.706	1.00 45.56
17	ATOM	5123	ō	HOH W 215	-2.433	36.012	80.232	1.00 54.12
35	ATOM	5124	ō	HOH W 216	5.257	25.271	55.914	1.00 53.23
93.44	ATOM	5125	ō	HOH W 217	13.354	64.403	53.862	1.00 33.23
	ATOM	5126	ō	HOH W 218	30.477	42.517	67.472	1.00 48.17
	ATOM	5127	ŏ	HOH W 219	14.139	47.479	76.123	1.00 79.04
	ATOM	5128	ō	HOH W 220	0.829	29.563	50.769	1.00 48.10
40	ATOM	5129	ō	HOH W 221	32.979	51.667	96.624	1.00 40.10
	ATOM	5130	ŏ	HOH W 222	14.677	45.948	71.756	1.00 52.31
	ATOM	5131	ō	HOH W 223	33.890	24.505	58.094	1.00 32.51
	ATOM	5132	õ	HOH W 224	17.853	9.519	65.560	1.00 45.05
	ATOM	5133	Ö	HOH W 225	37.794	31.473	62.305	1.00 50.38
45	ATOM	5134	ŏ	HOH W 226	29.206	50.335	62.673	1.00 45.43
	ATOM	5135	o.		4.932	48.808	63.354	1.00 43.45
	ATOM	5136	0	HOH W 228	18.933	59.070	55.899	1.00 50.29
	ATOM	5137	Ö	HOH W 229	13.849	18.833	83.641	1.00 55.89
	MOTA	5138	ŏ	HOH W 230	25.919	46.022	68.076	1.00 35.63
50	ATOM	5139	ŏ	HOH W 231	27.565	65.098	75.153	
. 50	MOTA	5140	ŏ	HOH W 232	27.128	39.012	68.497	1.00 73.11
	ATOM	5141	ō	HOH W 233	40.706	52.468	74.641	1.00 40.77 1.00 51.60
	ATOM	5142	o	HOH W 234	21.689	65.312		
	ATOM	5143	0	HOH W 235		17.615	58.080	1.00 66.72
55	ATOM	5144	0	HOH W 236	9.121 17.931		59.271	1.00 51.98
25	ATOM	5144	0	HOH W 237		36.565	88.091	1.00 54.77
					33.843	36.707	52.576	1.00 61.60
	ATOM	5146	0	HOH W 238	-3.693	50.074	63.986	1.00 43.64
	ATOM	5147	0	HOH W 239	44.272	44.279	81.461	1.00 69.21
60	ATOM	5148	0	HOH W 240	2.092	28.868	52.894	1.00 54.01
00	ATOM	5149	0	HOH W 241	8.309	33.518	71.442	1.00 68.05
	ATOM	5150	0	HOH W 242	1.051	31.947	69.204	1.00 52.88
	ATOM	5151	0	HOH W 243	44.255	51.162	96.650	1.00 20.00
	MOTA	5152	0	HOH W 244	16.173	45.408	46.636	1.00 20.00
	MOTA	5153	0	HOH W 245	41.130	50.734	97.991	1.00 20.00

5

5

CLAIMS

- 1. An isolated protein comprising at least a subsequence of the amino acid sequence of LTA₄ hydrolase, which exhibits a three-dimensional form essentially as disclosed in Table 9 by the parameters defining atom 1 to atom 4876, said subsequence being capable of participating in the control of the an enzymatic pathway, such as the leukotriene cascade, or a functionally equivalent part, derivative or conformational analogue thereof.
- 2. A protein according to claim 1, which comprises an enzymatically active site defined in the following table:

	Left wall	Right wall
1		Lys608, Asp606, Lys605, Lys354, Thr355
2	Phe356, Phe362	Gln544, Asp573, Lys572, Arg568
3	Val376	Lys565, Arg540, Leu507
4	Ser380, Ser352, Glu348	Pro569
5	Tyr378, Glu348	Arg563, Glu533, Phe536, Arg537, Tyr267
6	Tyr383, Phe314, Glu318, Glu384, Arg326	
7	Gly268, Gly269, Met270	His295, Asn341, Phe340
8	Ser288, His497	Glu325, Asn291

- 3. A protein according to claim 2, which is an enzyme having a metallohydrolase activity capable of participating in the regulation of enzyme activities in biochemical pathways, wherein said enzymes have structures similar to the ones defined in claim 2.
- A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Glu318; Tyr378; Tyr383; Arg563; Lys565.
- A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269;
 Met270; Glu271; Val292; His295; Glu296; His299; Trp315; Glu318; Val322:

- Phe362; Val367; Leu369; Pro374; Asp375; Ile372; Ala377; Pro382; Tyr378; Tyr383; Arg563; Lys565.
- A compound which is substantially complementary to a protein according to any one of claims 1-5.
- 7. A compound according to claim 6, which is substantially complementary to an enzymatically active site of said protein and which is capable of specifically inhibiting said enzymatic activity.
 - 8. A compound according to claim 7, which is an inhibitor of a metallohydrolase enzyme.
 - 9. An isolated complex, which is comprised of a protein according to claim 1-5 and a complementary compound according to any one of claims 6-8, wherein the three-dimensional structure of LTA₄ hydrolase is essentially as disclosed in Table 9 by the parameters defining atom 1- atom 4876, or a functionally equivalent part, derivative or conformational analogue of such a complex.
 - 10. A complex according to claim 9, wherein the protein complexed with LTA₄ hydrolase is selected from the group which consists of bestatin, thiolamine or hydroxamic acid, or a functionally equivalent part, derivative or conformational analogue of such a complex.
 - 11. Use of the parameters of a protein according to any one of claims 1-5, a compound according to any one of claims 6-8 or a complex according to claim 9 or 10 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry.
 - 12. Use according to claim 11, wherein said parameters are selected from the parameters disclosed in Table 9 defining atom 1- atom 4876.
- 25 13. Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or allergic symtoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS).
- 30 14. Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer.

30

- 15. Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 16. A method for screening LTA₄ hydrolase analogues that mimic at least a part of the three dimensional structure of the LTA₄ hydrolase molecule as defined by the parameters shown in Table 9 for atom 1 to atom 4876, which comprises the steps of
- (a) producing a multiplicity of analogue structures of LTA₄ hydrolase and
- (b) selecting an analogue structure, wherein the three-dimensional configuration and spatial arrangement of one or more enzymatically active sites and/or binding sites of said LTA₄ hydrolase remain substantially preserved.
- 17. A method according to claim 16, wherein an analogue exhibiting an enzymatic activity, such as an epoxide hydrolase and/or aminopeptidase activity, is selected.
- 18. A method according to claim 16 or 17, wherein an enzymatic inhibitor complementary to the amino acids defined in any one of claims 3, 4 or 5 is screened for.
- 19. An analogue obtainable by the method according to any one of claims 16-18.
- 20. An analogue according to claim 19, which exhibits an increased catalytic activity when compared to the naturally occurring form of LTA₄ hydrolase, such as defined in Table 9 by parameters of atom 1 to atom 4876.
- 21. A method for screening LTA₄ hydrolase binding compounds complementary to a region of LTA₄ hydrolase, preferably an enzymatically active site thereof, which comprises the steps of
 - (a) producing a multiplicity of possible complementary structures and
 - (b) selecting a structure, wherein the three-dimensional configuration and spatial arrangement of regions involved in binding to LTA₄ hydrolase remain substantially preserved, which selection is based on the three-dimensional structure of LTA₄ hydrolase, and/or LTA₄ hydrolase complexed to an inhibitor thereof, in a form adopted thereof in nature, such as defined in Table 9.
 - 22. A method according to claim 21, wherein a general metallohydrolase inhibitor is selected, which is capable of inhibiting an enzyme belonging to the M1 family.

- 23. A method according to claim 21, wherein an inhibitor of the epoxide hydrolase activity and/or aminopeptidase activity of LTA₄ hydrolase or of LTC₄ synthases is selected.
- 24. A method according to claim 21, wherein a compound capable of antagonizing LTB₄ receptor binding of a cell is selected.
- 25. A compound obtainable by the method according to any one of claims 21-24.
- 26. A method of engineering a protein, which method comprises the steps of
- -identification of a suitable set of mutations based on the structure of LTA₄ hydrolase;
- -generation of a library of genes which contains the suitable sequence variations;
- -selection of clones encoding the LTA₄ hydrolase analogues with a desired activity function;
 - wherein said desired activity is the capability of efficiently producing an organic compound of interest.
- 27. A method according to claim 26, wherein the specified property is the suicidal mode of action of LTA₄ hydrolase.
- 28. A process for the purification of a protein according to any one of claims 1-3 or obtained according to claim 26 or 27, which purification includes hydroxyapatite-based chromatography and a subsequent anion exchange chromatography.
- 29. A process for the crystallisation of an LTA₄ hydrolase, an analogue or a derivative thereof, wherein said crystallisation is performed with the addition of a ytterbium salt as an additive, such as an ytterbium chloride.
 - 30. A protein obtained by the method according to any one of claims 27-29.
 - 31. A protein according to claim 30, which is present in an essentially pure form.
- 25 32. An isolated nucleic acid encoding a protein according to claim 30 or 31.
 - 33. A nucleic acid capable of specifically hybridising to a the nucleic acid according to claim 32.
 - 34. Use of a protein, which is a genetically modified LTA₄ hydrolase, according to claim 30 or 31 in the preparation of LTB₄ or other metabolites in the leukotriene cascade.

- 35. A protein according to any one of claims 6-8, 25, 30 or 31 for use as a medicament.
- 36. Use of a protein according to any one of claims 6-8, 25, 30 or 31 in the manufacture of a medicament for the treatment and/or prevention of acute and chronic inflammatory and/or allergic disorders, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis and chronic obstructive pulmonary disease (COPD); neoplasias and/or cancer; or disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 37. Use of a protein according to any one of claims 6-8, 25, 30 or 31, in the manufacture of a medicament for the treatment and/or prevention of an anti-inflammatory and/or anti-allergenic disorder, such as bronchial asthma, allergic rhinitis, conjunctivitis etc.
- 38. Use of a protein according to any one of claims 6-8, 25, 30 or 31 in the manufacture of a medicament for the treatment and/or prevention of infection caused be human immunodeficiency virus (HIV).

Figure 1

Figure 2

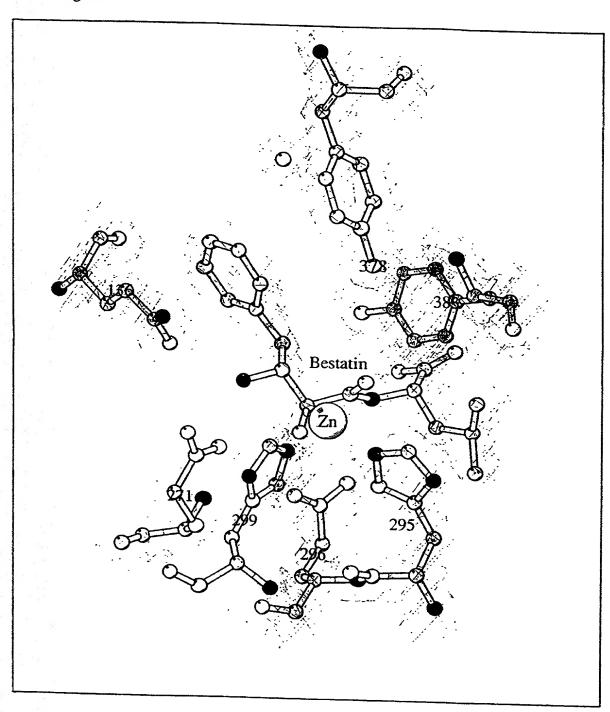
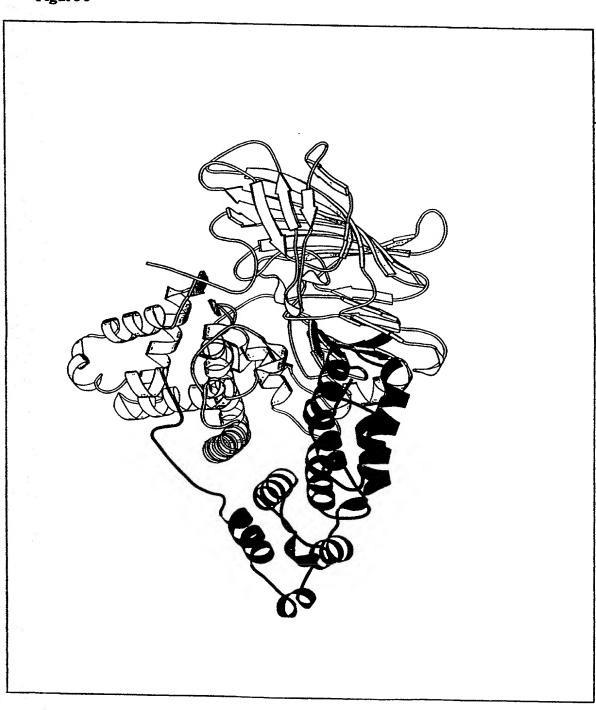
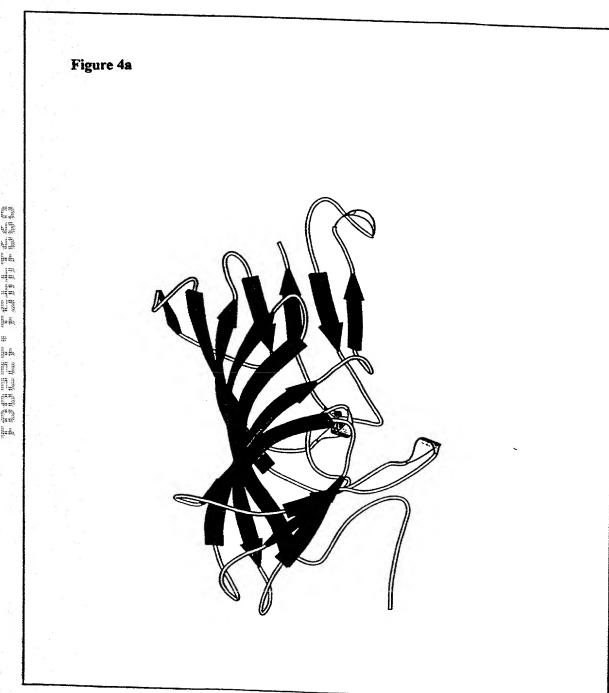
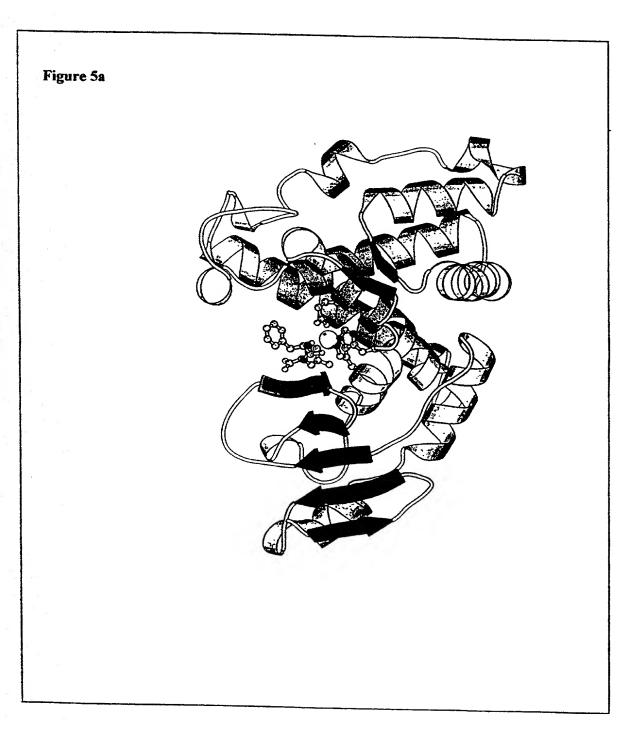


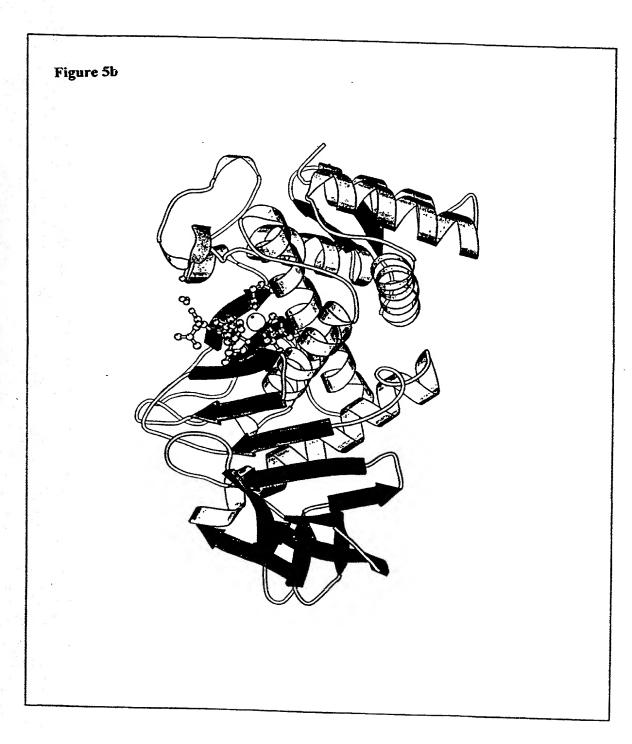
Figure 3











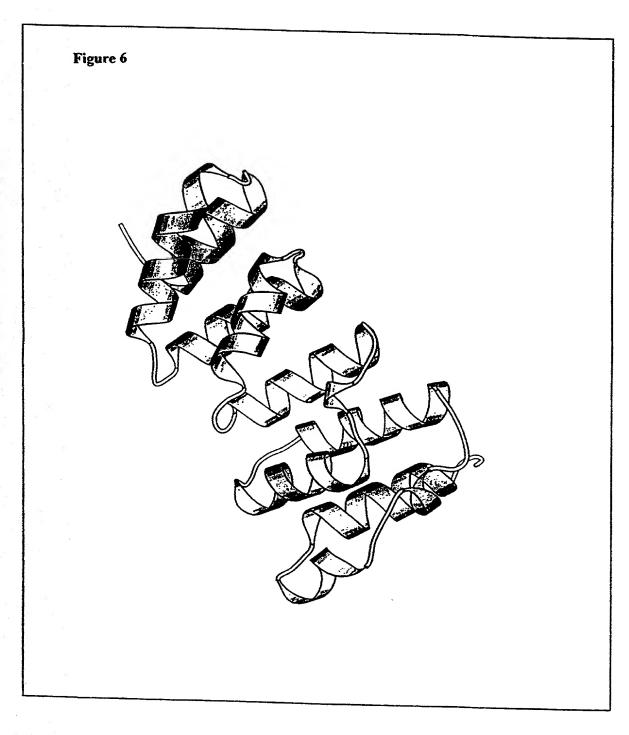
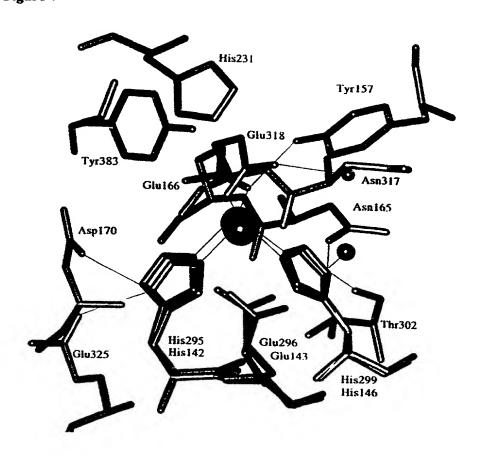


Figure 7



10/14

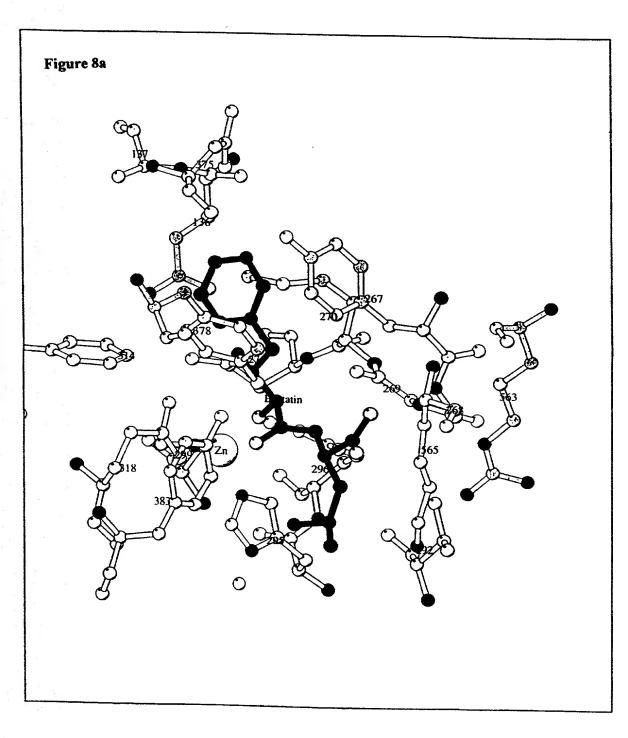
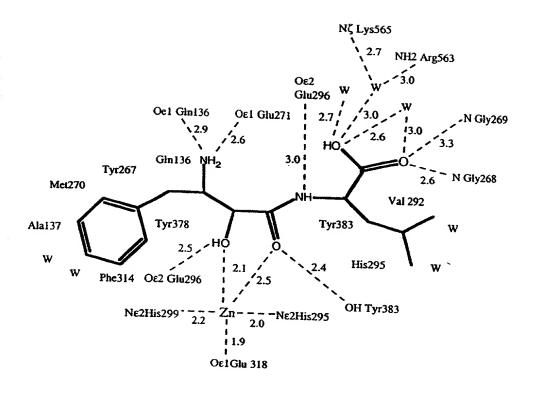


Figure 8b



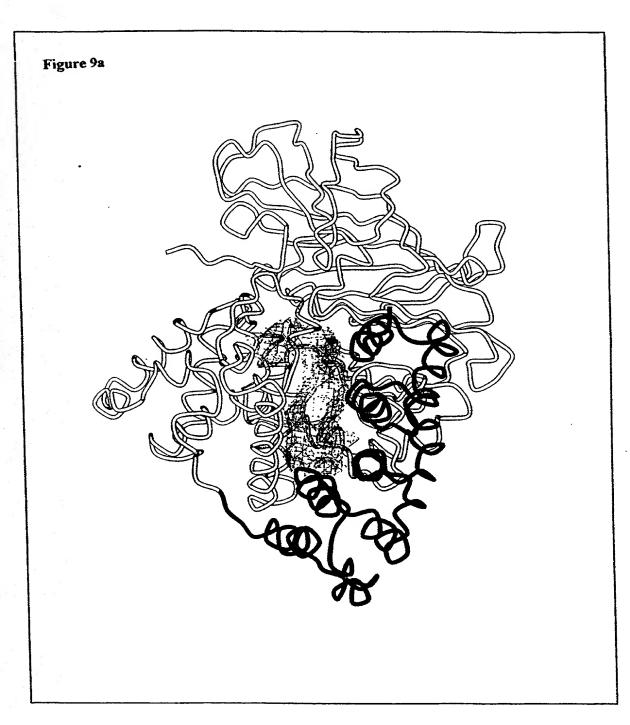
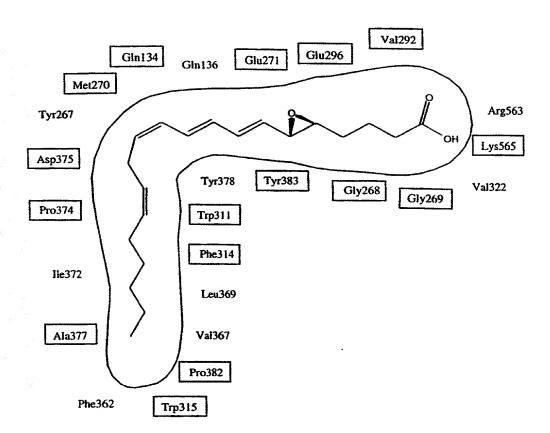


Figure 9b



DECLARATION, PETITION AND POWER OF ATTORNEY FOR PATENT APPLICATION

(Check	cone):				
X	Decla	ration Submitted with Initial Filing			
	Decla	ration Submitted after Initial Filing			
As a b	elow n	amed inventor, I hereby declare that:			
My res	sidence	e, post office address and citizenship are as stated below next to my name,			
origina	al, first	the original, first and sole inventor (if only one name is listed below) or an and joint inventor (if plural names are listed below) of the subject matter which do for which a patent is sought on the invention entitled:			
· ·	DRU	G DESIGN BASED ON THE STRUCTURE OF LTA4 HYDROLASE			
the spe	ecificat	tion of which (check one):			
	is attached hereto.				
:	OF	8			
×	was filed on 28 February 2000 as PCT International Application Number				
	PCT.	<u>/SE00/00384</u>			
		and was amended by PCT Article 19 Amendment on (if applicable),			
		and was amended by PCT Article 34 Amendment on (if applicable).			
to pate	entabil	ge the duty to disclose to the Office all information known to me to be material ity as defined in Title 37, Code of Federal Regulations, §1.56.			
ı nerek	ov state	e that I have reviewed and understood the contents of the above-identified			

specification, including the claims, as amended by any amendment referred to above.

PRIORITY CLAIM

(Check one):							
☐ no such applic	no such applications have been filed.						
such application	such applications have been filed as follows						
1) FOREIGN PRIOR States Code, §119(a)-(d §365(a) of any PCT inte United States of America application for patent or before that of the applic	or §365(b) of ernational applicational applications of the control	any foreign ap cation which of and have also ificate or any	pplicati designa identif PCT in	on(s) for patent ted at least one of the contract ted at least one of the contract ted below, by cl	or invente country of necking th	or's certific ther than th ne box, any	ate or ne foreign
Prior Foreign]
Application Number(s)	Application Date			Not Claimed	Yes	ached No	
9900722-1	SE	(mm,dd,yy 26 February (26.02.9	1999			×	-
		(20021)					1
2) PROVISIONAL PRO	ited States prov	visional applic	cation(s) listed below.		i, United S	tates
Provisional Application Number(s)			Filing Date (mm/dd/yyyy) 26 February 1999 (26.02.99)				
60/122,110			201 col uary 1999 (20.02.99)				
Additional provision hereto. 3) U.S./PCT PRIORIT §120 of any United State United States of America application is not disclose provided by the first part disclose information who of Federal Regulations, and the national or PCT	es application of a, listed below sed in the prior agraph of Title ich is known to §1.56 which be	hereby claim or §365(c) of a and, insofar a United States 35, United St ome to be mat came availabl	the ben any PCT s the su s or PCT ates Co terial to le betwe	efit under Title Ω Γ international a ibject matter of α Γ international a ide, §112, I ackn patentability as een the filing dat	35, United pplication each of the pplication owledge to defined in the policity of the policit	d States Con designating e claims of a in the manthe duty to n Title 37,	ode, ng the f this nner Code
U.S. Parent Application Number	PCT Parent 1	1		Filing Date d/yyyy)	1	Patent Nu plicable)	mber
					1,5,11		
a *							
☐ Additional U.S. or P sheet attached hereto.	CT internations	al application	numbe	rs are listed on a	suppleme	ental priori	ity

The Art of the Art of

POWER OF ATTORNEY:

As a named inventor, I hereby appoint the following attorneys and/or agents to prosecute this application and transact all business in the Patent and Trademark Office connected therewith.

James E. Cockfield	Reg. No. 19,162	Megan E. Williams	Reg. No. 43,270
Thomas V. Smurzynski	Reg. No. 24,798	Jeremiah Lynch	Reg. No. 17,425
Ralph A. Loren	Reg. No. 29,325	David J. Rikkers	Reg. No. 43,882
Giulio A. DeConti, Jr.	Reg. No. 31,503	Maria C. Laccotripe	Limited Recognition
Ann Lamport Hammitte	Reg. No. 34,858	-	Under 37 C.F.R. § 10.9(b)
Elizabeth A. Hanley	Reg. No. 33,505	Debra J. Milasincic	Reg. No. 46,931
Amy E. Mandragouras	Reg. No . 36,20 7	David R. Burns	Reg. No. 46,590
Anthony A. Laurentano	Reg. No. 38,220	Sean D. Detweiler	Reg. No. 42,482
Kevin J. Canning	Reg. No. 35,470	Peter S. Stecher	Reg. No. 47,259
Jane E. Remillard	Reg. No. 38,872	Cynthia L. Kanik	Reg. No. 37,320
Peter C. Lauro	Reg. No. 32,360	Theodore R. West	Reg. No. 47,202
DeAnn F. Smith	Reg. No. 36,683	Shayne Y. Huff	Reg. No. 44,784
Jeanne M. DiGiorgio	Reg. No. 41,710	•	

Send Correspondence to:

Elizabeth A. Hanley, Esq. Lahive & Cockfield, LLP, 28 State Street, Boston, Massachusetts 02109, United States of America

Direct Telephone Calls to: (name and telephone number)

Elizabeth A. Hanley, Esq., (617) 227-7400

Wherefore I petition that letters patent be granted to me for the invention or discovery described and claimed in the attached specification and claims, and hereby subscribe my name to said specification and claims and to the foregoing declaration, power of attorney, and this petition.

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

2	Full name of sole or first inventor
10	HAEGGSTRÖM, Jesper Z.
	Inventor's signature Date
	Expert 10eggs 2001-11-05
	Residence
	Valhallavägen 145, SE-115 31 Stockholm, SWEDEN
	Citizenship
	SE
100	Post Office Address (if different)

NORDLUND, Pär Inventor's signature	010	Date
150		2001-11-05
Residence	0	_1
Gruvbacken 2, SE-116 34 Stock	kholm, SWEDEN	EV
Citizenship		9
SE		

Full name of third inventor

THUNISSEN, Marjolein

Inventor's signature

Residence

Svinningevägen 26, SE-184 92 Åkersberga, SWEDEN

Citizenship

NL

Post Office Address (if different)

JC03 Rec'd PCT/PTO 2 7 AUG 2001

PCT/SE00/00384

WO 00/50577

SEQUENCE LISTING

	<u>022 </u>
<110> Haeggström et al	., Jesper
<120> DRUG DESIGN	BASED ON THE STRUCTURE OF LTA ₄ HYDROLASE
<130> 54660	
<140> <141>	
<160> 1	
<170> PatentIn Ver. 2.1	
<210> 1 <211> 611 <212> PRT <213> HUMAN	
<220> <223> AMINO ACID S HYDROLASE	EQUENCE OF HUMAN LEUKOTRIENE A4
<400> 1 Met Pro Giu Ile Val Asp 1 5	Thr Cys Ser Leu Ala Ser Pro Ala Ser Val 10 15
Cys Arg Thr Lys His Le	u His Leu Arg Cys Ser Val Asp Phe Thr Arg 5 30
Arg Thr Leu Thr Gly To	hr Ala Ala Leu Thr Val Gln Ser Gln Glu Asp 45
Asn Leu Arg Ser Leu V 50 55	al Leu Asp Thr Lys Asp Leu Thr Ile Glu Lys 60
Val Val Ile Asn Gly Gli 65 70	n Glu Val Lys Tyr Ala Leu Gly Glu Arg Gln 75 80
Ser Tyr Lys Gly Ser Pro 85	Met Glu Ile Ser Leu Pro Ile Ala Leu Ser 90 95
•	1 Ile Glu Ile Ser Phe Glu Thr Ser Pro Lys 05 110
Ser Ser Ala Leu Gln Tr 115 120	p Leu Thr Pro Glu Gln Thr Ser Gly Lys Glu 125
His Pro Tyr Leu Phe Se 130 135	r Gln Cys Gln Ala Ile His Cys Arg Ala Ile 140
Leu Pro Cys Gln Asp T 145 150	hr Pro Ser Val Lys Leu Thr Tyr Thr Ala Glu 155 160
Val Ser Val Pro Lys Gh 165	a Leu Val Ala Leu Met Ser Ala Ile Arg Asp 170 175

- Gly Glu Thr Pro Asp Pro Glu Asp Pro Ser Arg Lys Ile Tyr Lys Phe 180 185 190
- lle Gln Lys Val Pro Ile Pro Cys Tyr Leu Ile Ala Leu Val Val Gly
 195 200 205
- Ala Leu Glu Ser Arg Gln Ile Gly Pro Arg Thr Leu Val Trp Ser Glu 210 215 220
- Lys Glu Gln Val Glu Lys Ser Ala Tyr Glu Phe Ser Glu Thr Glu Ser 225 230 235 240
- Met Leu Lys Ile Ala Glu Asp Leu Gly Gly Pro Tyr Val Trp Gly Gln 245 250 255
- Tyr Asp Leu Leu Val Leu Pro Pro Ser Phe Pro Tyr Gly Gly Met Glu 260 265 270
- Asn Pro Cys Leu Thr Phe Val Thr Pro Thr Leu Leu Ala Gly Asp Lys 275 280 285
- Ser Leu Ser Asn Val Ile Ala His Glu Ile Ser His Ser Trp Thr Gly 290 295 300
- Asn Leu Val Thr Asn Lys Thr Trp Asp His Phe Trp Leu Asn Glu Gly 305 310 315 320
- His Thr Val Tyr Leu Glu Arg His Ile Cys Gly Arg Leu Phe Gly Glu 325 330 335
- Lys Phe Arg His Phe Asn Ala Leu Gly Gly Trp Gly Glu Leu Gln Asn 340 345 350
- Ser Val Lys Thr Phe Gly Glu Thr His Pro Phe Thr Lys Leu Val Val 355 360 365
- Asp Leu Thr Asp Ile Asp Pro Asp Val Ala Tyr Ser Ser Val Pro Tyr 370 375 380
- Glu Lys Gly Phe Ala Leu Leu Phe Tyr Leu Glu Gln Leu Leu Gly Gly 385 390 395 400
- Pro Glu Ile Phe Leu Gly Phe Leu Lys Ala Tyr Val Glu Lys Phe Ser 405 410 415
- Tyr Lys Ser Ile Thr Thr Asp Asp Trp Lys Asp Phe Leu Tyr Ser Tyr 420 425 430
- Phe Lys Asp Lys Val Asp Val Leu Asn Gln Val Asp Trp Asn Ala Trp
 435 440 445
- Leu Tyr Ser Pro Gly Leu Pro Pro Ile Lys Pro Asn Tyr Asp Met Thr 450 455 460
- Leu Thr Asn Ala Cys lle Ala Leu Ser Gln Arg Trp lle Thr Ala Lys 465 470 475 480
- Glu Asp Asp Leu Asn Ser Phe Asn Ala Thr Asp Leu Lys Asp Leu Ser

490

495

Ser His Gln Leu Asn Glu Phe Leu Ala Gln Thr Leu Gln Arg Ala Pro
500 505 510

Leu Pro Leu Gly His Ile Lys Arg Met Gln Glu Val Tyr Asn Phe Asn 515 520 525

Ala Ile Asn Asn Ser Glu Ile Arg Phe Arg Trp Leu Arg Leu Cys Ile
530 535 540

Gln Ser Lys Trp Glu Asp Ala Ile Pro Leu Ala Leu Lys Met Ala Thr 545 550 555 560

Glu Gln Gly Arg Met Lys Phe Thr Arg Pro Leu Phe Lys Asp Leu Ala 565 570 575

Ala Phe Asp Lys Ser His Asp Gln Ala Val Arg Thr Tyr Gln Glu His 580 585 590

Lys Ala Ser Met His Pro Val Thr Ala Met Leu Val Gly Lys Asp Leu 595 600 605

Lys Val Asp 610

PHURET ROS 20 DEC 2011

H'S

SEQUENCE LISTING

<110> Jesper Z. HAEGGSTRÖM et al.

<120> Drug design based on the structure of LTA4 Hydrolase

<130> 30630US02

<140> US 09/914,451

<141> 2001-08-27

<150> SE 9900722.1

<151> 1999-02-26

<150> US 60/122,110

<151> 1999-02-26

<160>1

<170> FastSEQ for Windows Version 4.0

<210>1

<211>610

<212> PRT

<213> homo sapiens

<400> 1

Pro Glu Ile Val Asp Thr Cys Ser Leu Ala Ser Pro Ala Ser Val Cys

Arg Thr Lys His Leu His Leu Arg Cys Ser Val Asp Phe Thr Arg Arg

Thr Leu Thr Gly Thr Ala Ala Leu Thr Val Gln Ser Gln Glu Asp Asn 35 40 45

Leu Arg Ser Leu Val Leu Asp Thr Lys Asp Leu Thr Ile Glu Lys Val 50 55 60

Val Ile Asn Gly Gln Glu Val Lys Tyr Ala Leu Gly Glu Arg Gln Ser 65 70 75 80

Tyr Lys Gly Ser Pro Met Glu Ile Ser Leu Pro Ile Ala Leu Ser Lys 85 90 95

Asn Gln Glu Ile Val Ile Glu Ile Ser Phe Glu Thr Ser Pro Lys Ser 100 105 110

Ser Ala Leu Gln Trp Leu Thr Pro Glu Gln Thr Ser Gly Lys Glu His 115 120 125

Pro Tyr Leu Phe Ser Gln Cys Gln Ala Ile His Cys Arg Ala Ile Leu 130 135 140

Pro Cys Gln Asp Thr Pro Ser Val Lys Leu Thr Tyr Thr Ala Glu Val 145 150 155 160

Ser Val Pro Lys Glu Leu Val Ala Leu Met Ser Ala Ile Arg Asp Gly 165 170 175

Glu Thr Pro Asp Pro Glu Asp Pro Ser Arg Lys Ile Tyr Lys Phe Ile 180 185 190

Gln Lys Val Pro Ile Pro Cys Tyr Leu Ile Ala Leu Val Val Gly Ala 195 200 205 Leu Glu Ser Arg Gln Ile Gly Pro Arg Thr Leu Val Trp Ser Glu Lys 210 215 220

Glu Gln Val Glu Lys Ser Ala Tyr Glu Phe Ser Glu Thr Glu Ser Met 225 230 235 240

Leu Lys Ile Ala Glu Asp Leu Gly Gly Pro Tyr Val Trp Gly Gln Tyr 245 250 255

Asp Leu Leu Val Leu Pro Pro Ser Phe Pro Tyr Gly Gly Met Glu Asn 260 265 270

Pro Cys Leu Thr Phe Val Thr Pro Thr Leu Leu Ala Gly Asp Lys Ser 275 280 285

Leu Ser Asn Val Ile Ala His Glu Ile Ser His Ser Trp Thr Gly Asn 290 295 300

Leu Val Thr Asn Lys Thr Trp Asp His Phe Trp Leu Asn Glu Gly His 305 310 315 320

Thr Val Tyr Leu Glu Arg His Ile Cys Gly Arg Leu Phe Gly Glu Lys 325 330 335

Phe Arg His Phe Asn Ala Leu Gly Gly Trp Gly Glu Leu Gln Asn Ser 340 345 350

Val Lys Thr Phe Gly Glu Thr His Pro Phe Thr Lys Leu Val Val Asp 355 360 365

Leu Thr Asp Ile Asp Pro Asp Val Ala Tyr Ser Ser Val Pro Tyr Glu 370 375 380

Lys Gly Phe Ala Leu Leu Phe Tyr Leu Glu Gln Leu Leu Gly Gly Pro 385 390 395 400

Glu Ile Phe Leu Gly Phe Leu Lys Ala Tyr Val Glu Lys Phe Ser Tyr 405 410 415

Lys Ser Ile Thr Thr Asp Asp Trp Lys Asp Phe Leu Tyr Ser Tyr Phe 420 425 430

Lys Asp Lys Val Asp Val Leu Asn Gln Val Asp Trp Asn Ala Trp Leu 435 440 445

Tyr Ser Pro Gly Leu Pro Pro Ile Lys Pro Asn Tyr Asp Met Thr Leu 450 455 460

Thr Asn Ala Cys Ile Ala Leu Ser Gln Arg Trp Ile Thr Ala Lys Glu 465 470 475 480

Asp Asp Leu Asn Ser Phe Asn Ala Thr Asp Leu Lys Asp Leu Ser Ser 485 490 495

His Gln Leu Asn Glu Phe Leu Ala Gln Thr Leu Gln Arg Ala Pro Leu 500 505 510

Pro Leu Gly His Ile Lys Arg Met Gln Glu Val Tyr Asn Phe Asn Ala
515
520
525

Ile Asn Asn Ser Glu Ile Arg Phe Arg Trp Leu Arg Leu Cys Ile Gln 530 535 540

Ser Lys Trp Glu Asp Ala Ile Pro Leu Ala Leu Lys Met Ala Thr Glu 545 550 555 560

Gln Gly Arg Met Lys Phe Thr Arg Pro Leu Phe Lys Asp Leu Ala Ala 565 570 575

Phe Asp Lys Ser His Asp Gln Ala Val Arg Thr Tyr Gln Glu His Lys 580 585 590

Ala Ser Met His Pro Val Thr Ala Met Leu Val Gly Lys Asp Leu Lys 595 600 605

Val Asp